Exploitation of a general-coordinate guiding centre code for the redistribution of fast ions in deformed hybrid tokamak equilibria.

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Abstract. Self-consistent fast ion distributions are usually obtained using a code that solves the guiding-centre equations, with an appropriate fast ion source (e.g. NBI pinis) and sink (e.g. collision operators). Straight field-line coordinate systems, such as Boozer coordinates, are ordinarily convenient due to the simple separation of longitudinal and cross-field motion, and the simple expression of magnetic differential operators. However, these coordinates are found to be near-singular at the boundary of the internal helical region associated with an \( n = m = 1 \) infernal mode. These important configurations are associated with many tokamak phenomena, including snakes and long-lived modes [1] in spherical or more conventional devices. Such internal helical states occur when there is a radially extended region where the safety factor is close to unity. Recent calculations predict the possibility of helical equilibria in ITER hybrid scenarios [2]. The ANIMEC code [3] conveniently produces an equilibrium helical state despite choosing for example an axisymmetric fixed boundary. The corresponding magnetic field in these coordinates can now be fed to the newly devised Particle-In-Cell (PIC) code VENUS-LEVIS, which has been upgraded with phase-space Lagrangian guiding-centre orbit equations [4], embodying full 3D anisotropic electromagnetic fields and a formulation that is independent of coordinate choice, despite retaining intrinsic Hamiltonian properties. The simulations are applied to MAST experiments where the presence of a long-lived mode can effect confinement of neutral beam ions, potentially affecting NBI heating and current drive [1]. Neighbouring equilibria from ANIMEC, one helical in the core and the other axisymmetric, permits a precise means of identifying the effect of 3D geometry on the simulated confinement properties of MAST’s neutral beam fast ion population. In agreement with the compared experimental data from MAST neutron camera, a significant fraction of particles are pushed out of the helical core region affecting both the measured radial neutron distribution and the heating and current drive properties of the neutral beam population.

1. Motivation

Modern fusion devices are nourished by powerful heating systems and operate at very energetic regimes. Large populations of non-thermal particles are produced, either via ICRH, NBI and/or \( \alpha \)-emission. Confinement of such fast particles is key to maintain plasma control and to avoid disruption.

Tokamak instabilities form non-trivial electromagnetic structure on top of which the motion of particles becomes complex and sometimes chaotic. Some instabilities will saturate at large amplitude and form stationary configurations. Despite the absence of electric fields, particle
orbits are again complex because of the 3D magnetic geometry. This is usually associated with loss of density, decrease of temperature and degradation of the conditions for fusion.

The study of fast ion transport is an important starting point for understanding the interplay between the fields and particles. Analytic progress has been made in simple cases, like axisymmetric geometry, linearized electromagnetic perturbations, simple fast ion distributions, etc., but it is necessary to treat more realistic situations, like helical tokamak core, Stellarator geometry, full-field perturbations (especially relevant for high beta plasmas), etc. For such investigations, numerical work becomes a necessity.

The \( n = m = 1 \) infernal mode consists of a helical displacement of the inner core region and is related to many Tokamak phenomena including snakes, long-lived modes in spherical or more conventional devices.

There is experimental evidence that such helical states strongly affect fast particles. This evidence is highlighted by neutron emissivity, which is directly related to ionization processes between fast ions and background deuterium/tritium. Observing MAST discharge with Long-lived mode (LLM)[1], it is found that the LLM develops as \( q_{\text{min}} \) approaches unity and correspondingly the neutron signal drops at a location assumed to be close to the magnetic axis. Then, when \( q_{\text{min}} \) crosses unity and the LLM fades away (equivalently the helical displacement shrinks), fast ion confinement is restored and the neutron signal returns to its initial intensity. It appears that the helical geometry is fully responsible for the expulsion of the hot particles out of the core region. Such interpretation begs for theoretical and numerical confirmation.

2. Model & Tools
A qualitative and quantitative estimate of the redistribution of NBI induced fast ions during a helical internal state is achieved by numerically solving the orbits about this particular magnetic configuration. The model assumes that a) the helical core is described as a static MHD equilibrium, and is unaffected by the fast ion distribution throughout the simulation\(^1\); b) spatial variation of the magnetic field is small with respect to Larmor radius of ions; c) plasma rotation is much slower than particle bounce motion but much faster than diagnostic and slowing-down time, i.e. equations of motion do not take into account centrifugal effects but particle deposition is randomized toroidally.

2.1. Guiding-centre drift equations
For the purposes of fast ion transport, it is arguably sufficient to consider the lowest order expansion in the guiding-centre approximation - the higher orders only being relevant for gyro-kinetics and the study of turbulence. Hence, the guiding-centre drift equations (GCDE) are derived by neglecting the particle’s fast and minute gyro-motion against the slow drift motion of the guiding-centre across the field-lines. It is equivalent to considering the first order magnetic moment \( \mu = mv_\perp^2 \gamma^2 / qB \) as being an adiabatic constant (and relativistic factor \( \gamma \) is defined below).

There are many approaches to derive the GCDE. The non-canonical phase-space lagrangian technique given by Littlejohn [4, 5] is especially suited for a general and coordinate independent formulation. Following his approach, we start with the relativistic guiding-centre phase-space Lagrangian

\[
\mathcal{L}_{\text{GC}}(X, \rho_\parallel, t) = (A + \rho_\parallel H) \cdot \dot{X} - \left( \frac{m}{q} c^2 \gamma + \Phi \right)
\]

\(^1\) The effect of energetic particles on the evolution towards a saturated helical state is not treated. While linear growth of the mode might be affected by fast ions, it is reasonable that the final saturated amplitude of the kink is not sensitive to the NBI population. In other words, the linear stage of the internal kink growth would be sensitive to FLR effects from the thermal ions and kinetic effects from the fast ions but the 3D equilibrium is not, especially for the cases considered here for which the pressure ratio \( P_{\text{hot}} / P_{th} \sim 5 – 10\% \).
where \( \mathbf{X} \) is the position of the guiding-centre, \( \rho_{||} \) is the parallel gyroradius (change of variable from \( v_{||} = \rho_{||} qH/mc\gamma \)), \( \mathbf{A} \) is the vector potential providing \( \mathbf{B} = \nabla \times \mathbf{A} \), \( \mathbf{H} = \sigma \mathbf{B} \) is the magnetic field intensity, permeability \( \sigma \) accounts for pressure anisotropy [6], \( \Phi \) is the electrostatic potential providing \( \mathbf{E} = -\nabla \Phi + \partial_t \mathbf{A} \) and \( \gamma \) is the relativistic factor carrying kinetic energy

\[
\gamma = \sqrt{1 + \frac{2 \mu B}{m c^2} + \frac{\rho_{||}^2 H^2}{(m/q)c^2}}
\]

The definition of parallel gyroradius was altered to include anisotropy explicitly. Since the phase-space Lagrangian does not contain a \( \dot{\rho}_{||} \) term, playing with its definition is transparent. This variable can be seen as a pivot variable to load physics in the GCDE (\( \mathbf{A}_{||} \) perturbations, plasma rotation,...). From (1), the Euler-Lagrange equations are derived and inverted to yield the following system of four differential equations as GCDE:

\[
\begin{align*}
\dot{\rho}_{||} &= -\partial \mathcal{H} \cdot \mathbf{B}^*/\mathbf{H} \cdot \mathbf{B}^* \\
\dot{\mathbf{X}} &= (v_{||} \mathbf{H} \mathbf{B}^* + \mathbf{H} \times \partial \mathcal{H}) /\mathbf{H} \cdot \mathbf{B}^*
\end{align*}
\]

where \( \partial \mathcal{H} = \frac{\mu}{q} \nabla B + v_{||} \rho_{||} \nabla H - \mathbf{E} + \rho_{||} \partial_t \mathbf{H} \) represents essentially the space-time gradient of the Hamiltonian.

It can be verified that these equations share the same conservation properties as those derived in the Hamiltonian canonical formalism, The underlying symplectic structure entails conservation of energy in time-independent cases, conservation of toroidal momentum in axisymmetric geometry, Liouville equation for phase-space volume, etc. These are essential for stable and consistent numerical implementation of guiding-centre motion. The vector equations of motion for \( \mathbf{X} \) highlights the freedom of choice in space coordinates and field representation.

2.2. **VENUS-LEVIS** orbit solver & PIC code

**VENUS-LEVIS** is an offspring of the **VENUS** code [7] rewritten in FORTRAN 90 to match performance, modularity and clarity criteria. Its primary function is to evolve particles solving the above GCDE (2), using a \( RK4 \) integrator scheme and fast linear interpolation of the field quantities over a tight 3D mesh. The choice of coordinate system and field representation is established via an independent *equilibrium module* loaded at compile time. Modules for straight field-line Boozer, **ANIMEC** [8] and **MINERVA** [9] coordinates are currently available.

Presently, **VENUS-LEVIS** is used as a particle-in-cell (PIC) code following an ensemble of weighted markers representing a slowing-down distribution of fast ions. An NBI module has been devised to provide the source of markers and a collection of Monte-Carlo operators, mimicking Coulomb collisions with background plasma, act as sinks [10]. The fields are not affected by the hot distribution and mutual interaction between fast particles is not taken into account.

The outcome of the code is a self-consistent estimation of the saturated fast ion distribution from NBI and the associated flux-averaged moments (fast ion density, pressure, current, etc.).

It is noted here that particular numerical challenges arise around the magnetic axis and near the transition region bounding the helical core. In particular, the magnetic axis is commonly accompanied by singularities in toroidal flux coordinate systems. A pseudo-cartesian patch combined with an analytic prescription of the fields partially overcomes this difficulty. In helical core equilibria this issue is enhanced by the geometrical spread of the magnetic axis and the large radial excursions of particles.

2.3. **ANIMEC** equilibrium solver

**ANIMEC** [8] is an equilibrium solver based on the premise that \( n = m = 1 \) instabilities eventually saturate into stationary internal helical core configurations satisfying the force balance equation.
These states are typically found for reversed-shear $q$-profiles with $q_{\text{min}} \sim 1$. The boundary, the pressure profile and the initial guess for the magnetic axis are prescribed to ANIMEC, which then uses an MHD-energy minimization principle to work out the 3D geometry of the flux surfaces and the components of the magnetic field. As is typical with root-finders, the bifurcation between axisymmetric and helical solution is very sensitive.

ANIMEC uses its own flux coordinate system - neither straight field-line nor orthogonal - resulting from the minimization of the Fourier spectrum. TERPSICHORE can be used to translate them into Boozer-like coordinates. Although straight field-line coordinates are more convenient to express field components (become flux quantities), perturbations and magnetic differential operators, the translation process is computationally heavy, as it requires a massive spectrum of modes. This is because Boozer coordinates end up being very contorted, if not singular, in the transition region between the helical core and axisymmetric mantle (see Fig. 1(a)).

On the other hand, the Jacobian of ANIMEC coordinates is close to zero near the transition region between helical core and axisymmetric mantle due to the packing of flux surfaces (see Fig. 1(b)). This leads to the spiking of some components of the field (currents) which is equivalently problematic.

3. Results

The tools described above were used to investigate numerically fast ion redistribution in MAST device. Based on experimental background profiles and plasma boundary measurements from MAST, ANIMEC was successful at recreating an axisymmetric and helical equilibrium. Markers, deposited in accordance with NBI pin in MAST, were evolved within VENUS-LEVIS and multiple snapshots of the resulting slowing-down distribution were taken to provide the statistics. A comparison between axisymmetric and helical situations is discussed below.

As a first result, it was observed that, on top of their usual radial drift, fast ions undergo large radial excursions from the inner helical core to beyond the transition region (see Fig. 2(b)). This implies that hot particles visit larger regions of the plasma and contribute to flatten the density profile. It is also noticed that many particles pass through the magnetic axis. This is a numerical difficulty because of the singular behaviour of flux coordinates. To avoid problems, it is possible to express the differential equations from polar (radial flux label $s$ and poloidal
Figure 2. In addition to their ordinary radial drift, passing particles undergo slower and larger radial excursion in helical geometry. This contributes to flattening the fast ion density profile near core region.

Figure 3. Fast ion density is reduced in helical core region.

angle $\theta$) to pseudo-cartesian variables $X = s \cos \theta, Y = s \sin \theta$. That way singular components for example $\partial B/\partial s \propto 1/\sqrt{s}$ entering in $\dot{\theta}$, are regularized by $s$. It is also essential that the interpolation scheme preserves the properties of the magnetic field\footnote{In the sense that $\nabla \cdot B = 0, \nabla \wedge B = K$, etc.}, so high-order interpolation or even analytic prescription are found useful.

Secondly, it is observed that the fast ion density profile drops proportionally to the helical displacement in the region around the magnetic axis (see Fig.3(a)). The toroidally averaged density decreases as well, but also flattens and broadens (see Fig.3(b)). This is a combined effect of the magnetic axis twisting around the torus and the orbits laying on larger portions of the equilibrium. These observations relate to the experimental data at a qualitative level. More simulations will be commissioned to answer more quantitative questions, especially for direct
comparison with MAST neutron emissivity data.

4. Conclusion

ANIMEC equilibrium solver is used to obtain $n = m = 1$ internal mode configuration, which is relevant for experimental plasmas and ITER hybrid scenario. Helical equilibria obtained from MAST configuration are fed to VENUS-LEVIS drift-kinetic solver to simulate energetic particle dynamics. Starting with an NBI source, the slowing-down distribution recovers the experimentally observed expulsion of fast ions from the central region where the helical mode is located. The derived guiding-centre drift equations provide a formulation of the problem that is independent of the choice of coordinates. This advantage is used to follow particles in the ANIMEC coordinate system, which is established to be smoother at the transition region between helical and axisymmetric mantel than the Boozer coordinate system. It is shown that hot particles have larger radial excursion in the helical core than in the axisymmetric configuration. Despite choosing a helical amplitude much smaller than that measured in MAST, the fast ion density in the core is significantly reduced. These ions are redistributed to the axisymmetric boundary, or lost from plasma entirely.

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