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Particle Modelling of Neoclassical Effects and Low-frequency Turbulence in Tokamak Plasmas

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Introduction

Investigation of particle and heat transport in tokamaks related to low frequency turbulence of either electrostatic or electromagnetic origin requires gyrokinetic two-component plasma simulation [1], including global equilibrium effects. Early 3-D particle simulations of dissipative trapped-particle instabilities in toroidal geometry [2] were limited to relatively short time with an unphysically small ion-electron mass ratio using eigenfunction expansion in toroidal geometry with a fairly small number of toroidal modes. Advancing ions in time with a gyrophase-averaged potential within a gyrokinetic formalism [1,3] has made it possible to extend the simulation range to cover ion dynamics scale and related instabilities. In a 3-D toroidal geometry, this has been possible so far practically only with adiabatic electrons, leaving out their kinetic effects, and by assuming time-independent background inhomogeneity [4-7]. Alternatively, in simulations with kinetic electrons flux tube domain has been applied making possible only local calculations. Common to these approaches has been the use of so called δf technique where only deviations from the given background are modelled. Although beneficial from the point of view of reduction of numerical noise in the early phase of instabilities in an otherwise quiet plasma, even some of its nonlinear extensions are still strongly based on fixed background not allowing global modifications in the particle distribution in configuration space and velocity.

In the present work, a full f gyrokinetic formalism is developed for its numerical implementation. Ions are advanced with a gyrophase-averaged electrostatic potential and electrons are under the influence of a bare potential. The ion polarization term in the gyrokinetic Poisson equation is calculated directly from a sampled particle distribution thus allowing strong non-Maxwellian deviations in velocity distributions and large deviations in background distribution. These amendments become of importance in integrating anomalous and neoclassical transport mechanisms in simulation. The new code, ELMFIRE, is a gyrokinetic version of the guiding-center orbit following Monte Carlo code ASCOT [8] which simulates only the neoclassical physics. Name ELMFIRE refers to long term goal to simulate dynamically ELMs and edge dynamics.

Full f model

Starting from the gyrokinetic formalism valid for ions linearly to arbitrary $k_\perp\rho$ and nonlinearly to $k_\perp\rho \leq 2$ [3], we derive a gyrokinetic Poisson equation

$$\nabla^2\Phi + \frac{2q}{\epsilon_0}\int \langle f\rangle_\alpha(\vec{x}-\vec{\rho},\mu,v_\parallel)\frac{1}{Bv_\perp}\frac{\partial\langle\Phi\rangle_\alpha(\vec{x}-\vec{\rho},\rho)}{\partial\rho}\frac{B}{2\pi}d\mu dv_\parallel d\phi = -\frac{1}{\epsilon_0}(q\tilde{n}_i - en_e), \quad (1)$$

suitable for numerical implementation with direct substitution from the gyrophased averaged guiding-center distribution function $\langle f\rangle_\alpha$ measured at $\vec{x}-\vec{\rho}$. In Eq.(1), $\Phi(\vec{x})$

is the electrostatic potential at the coordinate $\vec{x}$, $\tilde{n}_i$ and n_e are the ion and electron densities at $\vec{x}$, and $\langle\Phi\rangle_\alpha$ is a potential gyrophase averaged for an ion with a guiding-center at $\vec{x}-\vec{\rho}$ and a Larmor radius $\vec{\rho}=-\vec{v}_\perp\times\hat{b}/\Omega$. $\vec{k}$ is the wave vector of the mode, and $k_\perp$ is its perpendicular component with respect to the ambient magnetic field. $\mu=v_\perp^2/2B$ is the magnetic moment, $\vec{v}_\perp$ is the perpendicular ion velocity with repsect to the magnetic field $\vec{B}=B\hat{b}$, $\Omega=qB/m$ is the cyclotron frequency of the ion with a mass m and charge q. $v_\parallel$ is the ion parallel velocity, ϵ_0 is the vacuum permittivity, and e is the elementary charge. ϕ and α are gyrophases. In performing the partial derivative $\partial\langle\Phi\rangle_\alpha/\partial\rho$, $\vec{x}-\vec{\rho}$ is kept fixed.

In numerical implementation of Eq.(1), its right-hand side and the coefficient matrix for Φ in a given mesh constructed for $\vec{x}$ are calculated at each time step by sampling from the positions and weights of the simulation particles, ions and electrons, obtained by advancing the guiding-centers of the particles with a fourth order Runge-Kutta scheme. The guiding-center equations adopted, implementation of binary collisions to conserve momentum and energy between the particles, the fixed magnetic configuration, and the quiscent particle initialization method are as in ASCOT thus making possible to simulate neoclassical physics avoiding the limitations of the former methods. In sampling the coefficients of Φ and densities $\tilde{n}_i$ and n_e at $\vec{x}$ from the particle guiding-center positions $\vec{x}_{gc}=\vec{x}-\vec{\rho}$, nearest grid-point (NGP), cloud-in-cell (CIC), and subtracted dipole (SD) schemes have been tested. The particles have been assumed either as point-like or finite-size particles of equal size to the grid cell. Similarly, in calculating the force on particles from the potential, various orders of interpolation based on either point-like or finite-size particles have been tested. Four to 16 points on gyrocircles in gyrophase-averaging have been used.

A representative example of simulation domain is a radial shell of a torus with a shell width of some tens of ion gyroradii, but spanning more than 2-3 radial ion banana widths to eliminate unphysical boundary effects. In both radial and poloidal directions, grid cell size in the range between $(1...2)\rho$ has been selected. Quasi-ballooning coordinates [9] extending over the full magnetic surfaces are exploited making feasible long cell lengths along the magnetic field. Typically, $N_z=6-10$ cells in the toroidal coordinate are used. At the radial boundaries, gyro-circles extending outside the calculation domain are reflected back to the domain. Particles bringing their guiding-centers out of the domain are either reflected locally, with respect to the midplane, or are re-initialized at the boundary at hand. The re-initialization process is described in [8]. Here, it is used to either imitate the return ion flux against boundary losses and/or to set appropriate energy and particle sources at relevant boundaries.

In calculations with an adiabatic electron model where the electron density is obtained from $n_e=n_0[1+e(\Phi-\bar{\Phi})/k_BT_0]$ or from its nonlinear extension, the time step for particle guiding-center advancing is determined from ion dynamics, while with fully kinetic electron simulations, electron dynamics determines the shortest time step. Here, n_0 is an assumed reference density and T_0 a reference temperature for the electrons. In fully kinetic electron simulations, coefficient matrix of Φ in Eq.(1) and ion guiding-center advancing can be calculated with less frequent steps making large savings in CPU usage. On the other hand, electron advancing has been found to require iteration between the potential solving thus providing the strongest load on the code efficiency. An accurate electron time step is less than $\tau=2\pi R/(N_z v_T)$, where R is the

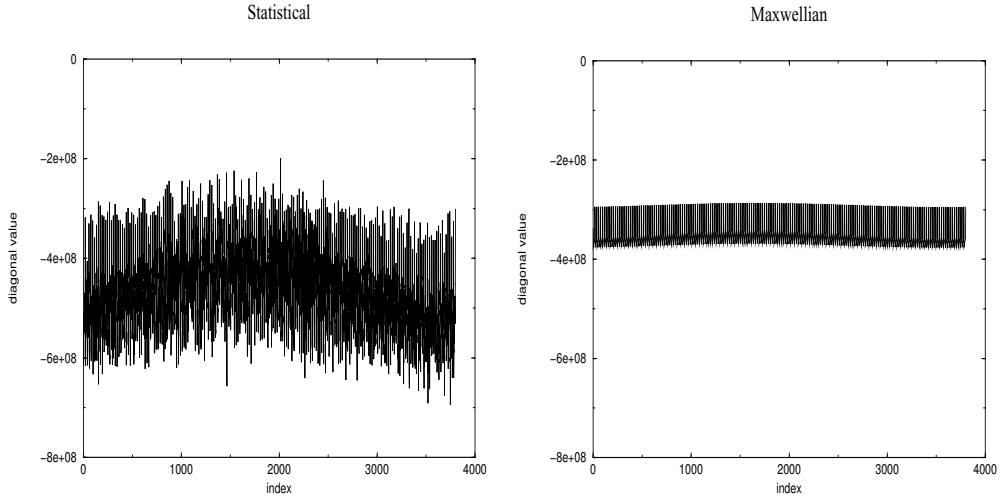

Figure 1: *The diagonal of coefficient matrix a) sampled from test particle ensemble b) from maxwellian distribution of particles*

major radius of the tokamak and v_T is the electron thermal velocity. For $R = 0.5$ m and $T_0 = 400$ eV, one has $\tau = 2 \times 10^{-8}$ s. Thus, on an ITG mode growth time of some tens of microseconds for typical plasma gradient conditions, thousands of time steps are needed for electron dynamics. With 2 million electrons, it takes 15 CPUs to advance and sample the electrons at each step for one iteration round. For a $N_r = 20$, $N_\chi = 200$, $N_z = 6$ mesh in the quasiballooning coordinate grid (r, χ, z) another 15 CPUs to calculate the potential on a Compaq AlphaServer ES45 computer is required at each iteration round. In δf technique, split-weight scheme allowing more efficient kinetic treatment of fast electrons has been recently developed which may relax the CPU usage even by an order of magnitude from the present approach. This method might be applicable in the present approach even not using δf technique for the ions.

Code validation

The new version of calculating the coefficient matrix in Eq.(1) has been tested against the conventional ion polarization term in Ref.[3] exploiting the Maxwellian velocity distribution. With a Maxwellian ion initialization, equal coefficient matrix has been found with these methods to the accuracy set by the noise in ion sampling. No deleterious effects from the point of view of numerical heating, stability, or accuracy in runs of 100 μs have been observed using the sampled coefficient matrix. Fig.1a shows the diagonal element of the coefficient matrix as a function of the grid index for the case: $a = 0.13$ m, $R = 0.36$ m, $B_T = 2$ T, $I = 0.14$ MA, $n_0 = 10^{19}$ m^{-3}, $T_0 = 400$ eV, $N_r = 20$, $N_\chi = 200$, $N_z = 6$. 960000 ions initialized in the calculation domain bounded by the radii $r_L = 0.07$ m, $r_R = 0.1$ m were used. Here, a is the plasma minor radius, R the major radius, B_T the toroidal magnetic field, and I the plasma current. The plasma is taken homogeneous with a parabolic current density profile. Circular cross-section with cocentric magnetic surfaces is assumed. In all three coordinates, the grid cells are equidistant. Initialization is performed with a Maxwellian distributed particles and zero potential. At the boundaries, the electrostatic potential is kept at zero value. No smoothing algorithm is applied. CIC technique in sampling and force interpolation was selected. The coefficient matrix is cumulated in sampling only over the time step Δt. $\Delta t = 2 \times 10^{-7}$ s was used with 8 points used for gyrophase averaging. In Fig.1b,

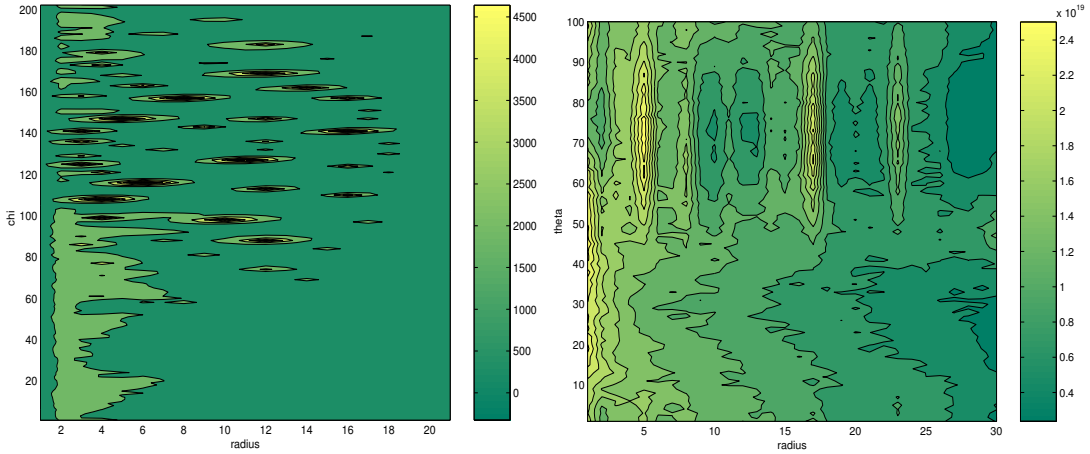

Figure 2: *a) Equipotential lines and b) ion density*

the diagonal element of the coefficient matrix for the analytically found matrix from the Maxwellian velocity distribution [9] is shown.

With the above parameters, the code has been run with adiabatic electrons. Fig.2 shows the equipotential lines at $t = 20$ μs in $(r-\chi)$ coordinates for the first toroidal grid cell at $z = \Delta z/2$ and the ion density averaged over toroidal angle in (r, θ) straight field line coordinates. It is found that the fluctuation levels mostly remain near the expected noise level $1/\sqrt{N_c}$, where $N_c = 40$ is an averaged number of ions in one cell. However, one can identify an appearance of convective cells and related density and potential peaks in the graphs, indicating a formation of turbulent dynamics from the noise. These structures were obtained with analytic coefficient but results with statistical coefficient matrix are essentially same. Possibe numerical origin of the peaking has been tested with different interpolation and sampling techniques [10] and further numerical analysis is still needed to clarify these issues. Potential peaking also slows down simulation if Δt is limited by $E \times B$ velocity. Filtering of the potential does not remove the peak formation but in many cases it makes simulation less CPU time consuming.

Summary

A new version of the ion polarization term in the gyrokinetic Poisson equation, feasible for direct and effective numerical implementation for global background dynamic variations, has been derived and tested. Together with fully kinetic treatment of electrons and with global calculation domain, this equation will be used for the analysis of electrostatic turbulence and neoclassical mechanisms in a consistent manner.

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