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**VENUS+ δf - A BOOTSTRAP CURRENT CALCULATION MODULE
FOR 3D CONFIGURATIONS**

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1. INTRODUCTION

The bootstrap current j_b is connected with collisional movements of the charged particles trapped in the local mirror fields. Many theoretical, numerical and experimental investigations for different tokamaks and heliotron-stellarators are devoted to the bootstrap current calculations.

For nonaxisymmetric toroidal systems there are several models and approaches. The problems are connected with the complicated 3D structure of the stellarator magnetic fields. The quasi-analytical fluid moment or so-called Shaing-Callen approach [1] has a compact semi-analytical form derived in [2]. This form (without the collisional dependence, for the low-collisional regime) constitutes the basis for several numerical tools with the self-consistent iterative equilibria - the SPBSC code [3] and the TERPSICHORE-BOOTSP code [4].

Another known approach for the bootstrap current calculations is the Drift Kinetic Solver DKES [5], used mainly with finite electrostatic potential. The DKES code was applied to the Wendelstein-7X device which has been optimised towards small bootstrap currents [6]. Another important application of the DKES code was for the National Compact Stellarator eXperiment [7] where up to the 50% of the rotational transform is provided by the bootstrap current.

In this paper, we present a new transport simulation tool - the VENUS+ δf - 3D code based on the VENUS [8] numerical orbits with a Monte Carlo technique used for the Lorentz collision operator and the δf weighting scheme for gyrokinetic particle simulation. The VENUS+ δf code calculates the diffusion coefficient and the bootstrap current j_b for the general 3D case and for any collisional regime without semi-analytical formulas and approximations conventionally applied in the DKES, SPBSC and TERPSICHORE-BOOTSP codes.

2. The δf EQUATIONS, IMPLEMENTED IN THE VENUS CODE WITH THE MOMENTUM CONSERVING MODEL FOR COLLISIONS

The original VENUS code uses as input the data describing fully 3D configuration parameters such as the magnetic field spectrum and the main flux values. This input is prepared initially by running the 3D equilibrium code VMEC [9] for given plasma boundary and by performing the further mapping to Boozer coordinates (S, θ, ζ) with

the TERPSICHORE [10] code. The numerical trajectories of charged particles are obtained from the guiding centre drift orbits equations solved with Runge-Kutta integrations scheme of second and the fourth orders with a fixed time step.

Collisions are taken into account using the Lorentz pitch angle scattering model based on the Monte Carlo technique [11] applied at each time step dt :

$$\lambda = \lambda_0(1 - \nu dt) + R[(1 - \lambda_0^2)\nu dt]^{1/2}, \quad (1)$$

where $\lambda = \frac{v_{\parallel}}{v}$ is the pitch angle variable, ν is a collision frequency, R - random number, $\langle R \rangle = 0, \langle R^2 \rangle = 1$.

In this paper we use the VENUS 3D numerical orbits in the so-called time varying weighting (δf) scheme developed initially for gyrokinetic particle simulation of neoclassical transport for tokamaks, see Refs. [12-14]. The starting drift kinetic Fokker-Planck equation for a guiding center distribution function f in a simple steady-state plasma with static magnetic field $B \mathbf{b}$ and no electric field has the form:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + (v_{\parallel} \mathbf{b} + \mathbf{v}_d) \nabla f = C(f), \quad (2)$$

where $C(f)$ is the collision operator. The distribution function in the expansion form $f = f_M + \delta f(t)$, where $f_M = f_M(S, E)$ - a local Maxwellian on the flux surface S , is substituted in the starting equation. The particle (marker) i with position $S_i(t)$ and with drift velocity $\mathbf{v}_{id}$ carries weight $\delta f_i(t)$ along the VENUS numerical trajectory. The equation for $\delta f_i(t)$ is:

$$\frac{d\delta f_i}{dt} = C(\delta f_i) - \mathbf{v}_{id} \cdot \nabla f_M, \quad d\delta f_i = -\Delta S_i \frac{df_M}{dS_i}, \quad (3)$$

This equation for $\delta f_i(t)$ is solved numerically in a special way. The change of weight $\delta f_i(t)$ is obtained after the collisionless step ΔS_i along the drift trajectory, then the pitch angle variable is changed in accordance with the collision operator (1). The average within the toroidal domain is defined as:

$$\langle A \rangle = \frac{\int A \delta f d\Omega}{\int f_M d\Omega} = \frac{\sum A_i \delta f_i d\Omega_i}{\sum f_M d\Omega_i} \quad (4)$$

To get the bootstrap current, one takes $A_i = v_{i,\parallel} = v_i \lambda_i$. The phase space volume of the marker i is $d\Omega_i = 2\pi v_i^2 dv_i d\lambda_i \sqrt{g_i} dS_i d\theta_i d\zeta_i$, here the Boozer jacobian $\sqrt{g_i}(S_i, \theta_i, \zeta_i)$ is a time dependant function that varies along the trajectory of the marker.

In the VENUS+ δf code, we use the Lorentz collision operator with momentum conservation for like-particle collisions, ν - the collision frequency, u - flow velocity:

$$C(f) = \frac{\nu}{2} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \left(\frac{\partial f}{\partial \lambda} - 3f \frac{u}{v} \right) \quad (5)$$

Momentum conservation is achieved in a second step by changing the marker particle weights δf_i by a correction term. For N_p monoenergetic particles, to conserve the parallel momentum, the correction term has the form [15]:

$$\Delta \delta f_i = \frac{3u}{v} f_M \lambda \nu dt, \quad u(s, \theta) = \sum \frac{\delta f_i}{f_M} \frac{v_{i,\parallel}}{N_p}. \quad (6)$$

To verify the conservation of the parallel momentum $\langle u \rangle$ and the number of particles $dN = \sum \delta f_i d\Omega_i$, we consider a model without drifts, $\sqrt{g_B} = 1$, taking into account only the pitch angle scattering with the initial condition $\delta f_i = (c_1 \lambda_i + c_2) f_M$.

Fig.1

The normalized momentum versus the time step with different number of particles for the case $\nu dt = 0.001$ is presented in Fig. 1. For the case $\nu dt = 0.1$ with $N_p = 10^6$ particles, the statistical error is less than 1%. Several other momentum and particle number conservation tests with the VENUS+ δf code confirm that the statistical error σ can be decreased according to the law $\sigma \approx N_p^{-1/2}$. It was shown also that the momentum conservation leads to a δf linear in the pitch angle variable.

3. RESULTS FOR THE JT-60 TOKAMAK AND THE W7X STELLARATOR

To perform the comparison with the well known analytical theory, we calculated with the VENUS+ δf code the diffusion and the bootstrap current for the different collisional regimes at a plasma radius $r = 0.42$ m in the JT-60 tokamak with minor and major plasma radii of 1.0 m and 3.0 m, respectively. Good agreement of the VENUS+ δf code with the analytical theory for the Pfirsch-Schluter, plateau and banana regimes $j_b \approx (1 + \sqrt{\nu_*} + 1.44\nu_*)^{-1}$ is shown on Figure 2. The calculations were done using energy convolution. The same comparison has been performed for the diffusion coefficient.

Fig.2

We have investigated also with the VENUS+ δf code the so-called "local" approach, proposed in Ref. [16]. The idea of this local approach is to return the marker after each time step onto the initial surface with the same poloidal and toroidal angles. However, each step gives the contribution to the particle weight according to equation (4). The local approach gives the same result as full trajectory runs if the orbits are located mainly near the initial surface.

For the comparison of the VENUS+ δf code results for the non-axisymmetric case, we calculate the monoenergetic bootstrap current coefficient D_{31}^* , normalized to the limiting value of the equivalent axisymmetric tokamak with circular flux surfaces. The typical time history of the bootstrap current coefficient for particles starting at half the plasma radius in the W7X stellarator is shown in Fig. 3.

Fig.3

Here one can see two different levels of the bootstrap current obtained for an inverse mean free path $\nu/V = 10^{-4}[1/m]$ with the DKES code (upper level) [17] and with the Shaing-Callen analytic formula (lower curve). An exponential least-squares fit of the

VENUS+ δf code results gives the same result for the bootstrap current coefficient as the DKES code.

As demonstrated in Ref. [18] for the very long-mean-free-path *lmfp* regime, the W7X stellarator ripple trapped particles have rapidly increasing weights. For these particles, the main expansion assumption $\delta f_i \ll f_M$ is violated and the solution is not steady-state. To conserve the number of particles and to fulfill the assumption $\delta f_i \ll f_M$, we investigate with the VENUS+ δf code the new procedure for such markers - the return of the particles (the markers with large δf_i) with zero weight. It has been shown that this procedure yields the steady-state solution for the *lmfp* regime.

Fig.4

Fig. 4 presents the bootstrap current coefficient D_{31}^* , plotted as a function of inverse mean free path, obtained with the DKES code and with the VENUS+ δf code with the new procedure for the markers with large weights. For comparison purposes, the D_{31}^* coefficient in the collisionless limit of the Shaing-Callen approach is plotted as a constant line independent of ν/V . In this plot, we show the results of the VENUS+ δf code for particles with the same energy $E = 100\text{eV}$, but with different atomic mass ($A = 0.2; 2; 20$). It is clearly seen from Figure 4 that small gyroradius (normalized to the minor radius of the initial position r_{start} , $\rho/r_{start} = 0.02$ for particles with atomic mass $A = 0.2$) exactly corresponds to the DKES results. Heavy ions with $A = 20$ and $E = 100\text{eV}$ have larger gyroradius and produces smaller bootstrap current coefficients.

The main VENUS+ δf calculations were performed on the pleiades.epfl.ch Linux cluster. This cluster has 132 Pentium 4 processors with 2.8GHz and 2Gb. For the very *lmfp* regime, $\nu/V = 3 * 10^{-6} [1/m]$, the new multi-processor VENUS+ δf version with 48000 particles makes 10^6 steps on 6 processors during ≈ 91 hours.

4. SUMMARY

We have described the new neoclassical code VENUS+ δf - based on the VENUS numerical orbits with the implementation of the δf equations for the bootstrap current and

the diffusion coefficient calculations. An accurate drift orbit solver in fully 3D coordinates permits to consider both tokamak and stellarator configurations and to take into account pitch angle scattering collisions with momentum conservation.

Several successful tests and benchmarks have been performed for the JT-60 tokamak and the W7X stellarator, including the main conservation tests, the convergence study and the dependence of the diffusion coefficient and the bootstrap current versus the collision frequency and poloidal angle.

In the near future, we plan to include in the VENUS+ δf code the electric field effects; the full Landau collision operator; thermalisation (not only pitch angle scattering and momentum conservation); the dependence on the density and the temperature profiles (scan in S -profiles). We hope also to compare the VENUS+ δf code with other tools and with the experimental results for tokamaks and stellarators (W7X, LHD, NCSX) within the different international collaborations.

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