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

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Abstract

We present a new 3D code - VENUS+δf - for neoclassical transport calculations in nonaxisymmetric toroidal systems. Numerical drift orbits from the original VENUS code and the δf method developed for tokamak transport calculations are combined. The first results obtained with VENUS+δf are compared with neoclassical theory for different collisional regimes in a JT-60 tokamak test case both for mono-energetic particles and for a Maxwellian distribution; good agreement is found. Successful benchmarking of the bootstrap current in the W7-X configuration with the DKES code for different collisionality regimes as well as further VENUS+δf developments are described.

1. INTRODUCTION

The bootstrap current j_b is connected with collisional movements of the charged particles trapped in local mirror fields. This current arises from the asymmetric transfer of parallel momentum due to the radial drift of trapped particles.

Many theoretical, numerical and experimental investigations for different tokamaks and stellarators/heliotrons are devoted to the bootstrap current calculations. For example, analytical neoclassical theory[1] yields for tokamaks in the paraxial approximation (the minor plasma radius r is much smaller than the major plasma radius R) the relation: $j_b = f_t \cdot \frac{1}{B_p}\frac{dp}{dr}$, where $f_t \simeq 1.46\sqrt{\frac{r}{R}}$ is the trapped particle fraction, p is the plasma pressure, and B_p is the poloidal magnetic field. More generally, as a numerical example, the CQL3D code[2] computes neoclassical transport coefficients for general axisymmetric equilibria for arbitrary collisionality regimes.

For nonaxisymmetric toroidal systems, there are several models and approaches. The problems are connected with the complicated 3D structure of the stellarator magnetic fields. One quasi-analytical fluid moment, the so-called Shaing-Callen approach[3], has a compact semi-analytical form derived in Ref. 4. This expression, describing the collisionless asymptote, i.e. the bootstrap coefficient becomes independent of collisionality, is the basis for several numerical tools with self-consistent iterative equilibria, e.g. the SPBSC code[5] (NIFS, Japan) and the TERPSICHORE-BOOTSP code[6] (CRPP, Switzerland). With both codes, the impact of the bootstrap current on the MHD stability can be analyzed for quite different magnetic configurations. Successful benchmarks of these fluid moment model codes for JT-60, W7-X and LHD configurations were reported in Ref. 7.

Another existing approach for bootstrap current calculations is the Drift Kinetic Equation Solver, DKES[8], used mainly with finite radial electric field. The DKES code was applied for the Wendelstein-7X (W7-X, Greifswald, Germany) device, which has been optimized towards small bootstrap currents[9]. Another important application of the DKES code was for the National Compact Stellarator eXperiment[10] (NCSX, PPPL, USA), where up to the 50% of the rotational transform is provided by the bootstrap current, which might affect the MHD stability properties. For very low collisionalities, i.e. deep in the long-mean-free-path (*lmfp*) regime, the $1st$ order distribution function becomes highly localized close to the passing - trapped particle boundary with increasing radial electric field. For these conditions, DKES usually provides transport coefficients with large uncertainties depending on the specific magnetic configuration. Furthermore, no solution can be obtained by DKES for fairly large radial electric fields.

The discrepancy between the DKES code and the Shaing-Callen approach for the W7-X bootstrap current in the *lmfp* regime is about a factor of 2.5 and has been reported in Ref. 11. This difference can be attributed to a combination of the approximations made in the quasi-analytic approaches and the effects of the collision operator. So, neoclassical calculations for stellarators in the different collisionality regimes, in particular for the *lmfp* regime, remain an important task.

The bootstrap current can affect the MHD equilibrium properties by causing low-order resonant magnetic surfaces within the plasma. In this sense, the bootstrap current might provide a free energy source for destabilizing (global) ideal MHD kink modes in the vicinity of these rational surfaces. Furthermore, an island divertor configuration with a low order-rational rotational transform at the separatrix is significantly affected even by small bootstrap currents which must be controlled in order to allow for an efficient divertor operation (this is the case for W7-X). These examples provide motivation for a reliable estimation of the bootstrap current.

In this paper, we present a new tool - the VENUS+δf - 3D code based on the VENUS[12] numerical orbits, the 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 all collisionality regimes without semi-analytical formulas and approximations applied in the DKES, SPBSC and TERPSICHORE-BOOTSP codes.

The paper is organized as follows. Section 2 describes the recent update of the VENUS code which implements the additional control parameters and the δf equations for the neoclassical transport calculations. Section 3 shows the neoclassical transport results with this code for the standard tokamak JT-60 and Section 4 describes the VENUS+δf results for the advanced stellarator W7-X including a new *lmfp* weighting procedure, the benchmark with the Shaing-Callen approach and with DKES results. In the Summary, the main results and future plans are discussed.

2. The δf EQUATIONS IMPLEMENTED IN THE VENUS CODE.

The original VENUS code uses as input the data fully describing 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[13] for a given plasma boundary and by performing an additional mapping to Boozer coordinates (ψ, θ, φ) with the TERPSICHORE[14] code. The numerical trajectory of a charged particle is obtained from the guiding center drift orbit equations which are solved with Runge-Kutta integration schemes of second and fourth orders with fixed time steps.

Collisions are taken into account by using the Lorentz pitch angle scattering model based on the Monte Carlo technique[15], which is applied at each time step, dt:

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

where $\lambda = \frac{v_{\parallel}}{v}$ is the pitch variable, λ_0 is the pitch prior to the collision event, ν is the collision frequency, and R a random number with $< R >= 0, < R^2 >= 1$. This model generates stochastic trajectories for different collisionality regimes provided that $\nu dt <<$ 1. The complete simulation time, τ, should include several collision times, $\nu\tau > 1$. For the *lmfp* regime, these constraints require a large number of time steps dt.

In this paper, we use the VENUS 3D numerical orbits using the time varying weighting (δf) scheme developed initially for gyrokinetic particle simulations of neoclassical transport for tokamaks, see Refs. 16-18. The starting drift kinetic Fokker-Planck equation for the guiding center distribution function f in a steady-state plasma with static magnetic field $B\,\boldsymbol{b}$ with $\boldsymbol{b}$ the unit vector in the direction of $\boldsymbol{B}$ and without a parallel electric field (loop voltage) has the form:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + (v_{||}\boldsymbol{b} + \boldsymbol{v_d})\nabla f = C(f), \tag{2}$$

where $C(f)$ is the collision operator and the velocity space variables are total energy and magnetic moment, both being invariant during the collisionless motion. The distribution function in its expanded form $f = f_M + \delta f$, with $f_M = f_M(\psi, E)$ the local Maxwellian on the flux surface ψ, is substituted in Equation 2. Here, the basic small expansion parameter is ρ/r, where ρ is the gyroradius and r is the minor radius. The particle (marker) i at the magnetic surface $\psi_i(t)$ and with the drift velocity $\boldsymbol{v_{di}}$ carries a weight $\delta f_i(t)$ along the VENUS numerical trajectory. The first order equation - the equation for $\delta f_i(t)$ is:

$$\frac{d\delta f_i}{dt} = C(\delta f_i) - \boldsymbol{v_{di}} \cdot \boldsymbol{\nabla} f_M, \tag{3}$$

This equation for $\delta f_i(t)$ is solved numerically. The change of the weight, $\Delta\delta f_i(t)$, is obtained after the collisionless step $\Delta\psi_i$ along the drift trajectory:

$$\Delta\delta f_i = -\Delta\psi_i \frac{df_M}{d\psi_i}, \tag{4}$$

and the pitch variable is changed according to the collision operator (1). The average procedure is defined as

$$< A >= \frac{\int A\delta f d\Omega}{\int f_M d\Omega} = \frac{\sum A_i \delta f_i d\Omega_i}{\int f_M d\Omega}. \tag{5}$$

To get a measure of the bootstrap current, one takes $A_i = Bv_{||,i} = Bv_i\lambda_i$. In the $v, v_{||}, \psi, \theta, \varphi$ phase space variables, the phase space volume of the marker i is given by

$$d\Omega_i = 2\pi v_i^2 dv_i d\lambda_i \sqrt{g}_i d\psi_i d\theta_i d\varphi_i, \tag{6}$$

where the Boozer Jacobian $\sqrt{g}_i(\psi_i, \theta_i, \varphi_i)$ is a function of the particle position, i.e. a local quantity, varying along the trajectory of the marker i. At the beginning of the calculations, a uniform Maxwellian or, in an option with less statistical noise, a series of monoenergetic ensembles of electrons or of ions is loaded on a prescribed starting magnetic surface, and is randomly distributed with respect to the poloidal, toroidal and pitch angle variables. Vanishing weights are taken as initial conditions, which is equivalent to assuming the initial distribution is Maxwellian. A steady-state solution for the bootstrap current is observed after several collisional times [16-18].

Accurate collision operators conserving momentum and energy for like-particle collisions in electron-ion plasmas for gyrokinetic simulations are given in Ref. 16. We plan to present in the near future the VENUS+δf results using the modified Lorentz collision model with momentum conservation.

3. RESULTS FROM VENUS+δf FOR THE JT-60 TOKAMAK

To perform the comparison with the well-known analytical theory, we calculated with VENUS+δf the diffusion and the bootstrap current for the different collisionality regimes at a plasma radius $r = 0.42$ m in the tokamak JT-60 with minor and major plasma radii 1.0 m and $R_0 = 3.0$ m, respectively. The typical time history of the bootstrap current near the plateau regime for the case with $\nu^* = 0.26$ is shown in Figure 1. The dimensionless collisionality, ν^*, is defined following Ref. 16 by $\nu^* = (r/R_0)^{-3/2}\nu\sqrt{2}R_0/(\iota V)$, where V is the thermal velocity. As expected, stationary conditions with a small statistical error are reached after 5-10 collisional times both for the plateau and for the banana regime.

Good agreement of the VENUS+δf code with the analytical bootstrap current[1] using the simplified Lorentz collision model for the Pfirsch-Schlüter, plateau and banana regimes $j_b = j_{b0}/(1 + \sqrt{\nu^*} + 1.44\nu^*)$ is shown in Figure 2. The calculations were performed with energy convolution as in Ref. 8, i.e. we quantify the contributions of particles with different energies in accordance with the Maxwellian distribution law.

The comparison with the analytical particle flux, proportional to the diffusion coefficient, is shown in Figure 3. In this case, again, a simplified Lorentz collision model is used to calculate the analytical particle flux. Good agreement of the VENUS+δf result with the analytical poloidal dependence of the current distribution for the Pfirsch-Schlüter regime is demonstrated in Figure 4. For the plot of the poloidal distribution of the local bootstrap current, we divide the poloidal angle into $m_{pol} = 40$ equal bins and calculated the fraction of the current $j_b(\theta_i)$ in each bin. Consequently the averaged current is calculated according to $< j_b >= \sum j_b(\theta_i)/m_{pol}$. To obtain low statistical errors for the poloidal distribution through the binning process, we need a larger number of particles. For the bootstrap current calculation, which is the average, one needs significantly less particles.

With VENUS+δf we have also investigated the so-called "local" approach, proposed in Ref. 20. 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 in accordance with equation (4). The local approach should give the same result as the full solution for conditions where particles do not depart too much from their birth surface. Figure 5 confirms the equivalence of the local approach (no radial drifts) and full trajectory (with radial drifts) runs.

4. RESULTS FROM VENUS+δf FOR THE W7-X STELLARATOR

The mono-energetic electron or ion bootstrap current is $j_{be,bi} = \Delta_0 D^*_{31} dp_{e,i}/dr$ (see Ref. 1) with the bootstrap current coefficient, D^*_{31}, normalized to the collisionless asymptote, $\Delta_0 = 0.9733\sqrt{R/r}/(\iota B_0)$, of an equivalent large-aspect-ratio tokamak with circular cross section. Energy convolution with the Maxwellian distribution function yields the factor 1.46 (compare Ref. 1) instead of 0.9733. For the comparison of VENUS+δf results for non-axisymmetric cases, we calculate the normalized mono-energetic coefficient D^*_{31}. Here, we consider the "standard" configuration[11] (referred to as "sc1") of the stellarator W7-X.

A typical time history of the bootstrap current coefficient for particles starting at half of the plasma radius in W7-X is shown in Figure 6. Here one can see two different levels of the bootstrap current obtained for the inverse mean free path $\nu/V = 10^{-4}[1/m]$ with the DKES code (upper level) [11] and with the Shaing-Callen analytic formula (lower curve). An exponential least-squares fit of the VENUS+δf code results as obtained with the procedure described below gives the same result for the bootstrap current coefficient as DKES.

As reported in Ref. 21, the ripple-trapped particles in stellarators can have rapidly increasing weights reflecting the advantage of the δf-scheme for radial particle transport simulations, in particular in the very-*lmfp* regime. This is different to the tokamak case where the weights δf_i are periodic functions without collisions. Those ripple-trapped particles with large δf_i, however, have only a small contribution to the bootstrap current (which is mainly determined by barely trapped and barely passing particles), but have a very negative impact on the statistical properties of the δf-scheme. Furthermore, the smallness assumption $\delta f_i << f_M$ can be violated and a stationary result cannot be obtained. Markers with rapidly increasing weights can be considered as lost particles. To conserve the number of particles and to fulfill the assumption $\delta f_i << f_M$, we implemented in the VENUS+δf code a new procedure for such markers - the replacement of "lost particles" (i.e. markers with e.g. $\delta f_i > 0.01 f_M$) with zero weight which corresponds to maintaining the Maxwellian on the start surface. It was shown with different numbers of particles and for the different values of the inverse mean free path that this procedure gives a steady-state solution for the very-*lmfp* regime.

In VENUS+δf bootstrap current simulations, "lost particles" are handled in the following way: First they are identified by the magnitude of their weight δf_i exceeding a numerical bound, e.g. 1% of the background distribution f_M. These markers are then replaced in the simulation on the same magnetic surface, but with $\delta f_i = 0$. In this way, conserving the number of markers, the statistical properties of the δf-scheme are not degraded. New weights ($\delta f_i = 0$) reduce the small contribution of ripple-trapped particles with strong radial drift to the estimation of the bootstrap current coefficient. One clearly needs to make sure that the numerical bound is indeed not set too low so as to affect the final result.

For magnetic configurations without significant drift-optimization and for small radial electric field ($1/\nu$-regime), ripple-trapped particles are replaced after a much shorter time compared to drift-optimized configurations or with a sufficiently large radial electric field. Consequently, the $|\delta f_i|$-bound should be fairly equivalent for the different scenarios.

From the marker eq. (4), one obtains directly an averaged relation between the bound for $|\delta f_i|$ and the maximum radial displacement due to the radial drift of the ripple-trapped particle. Consequently, this "filter" technique based on $|\delta f_i|$-bounds is equivalent to the one described in Ref. 19: "If a particle leaves the narrow ψ annulus, the event is recorded and the particle is put back into the middle of the annulus". A more detailed analysis of this "filter" effect on the D^*_{31} estimation with respect to the $\delta f_i/f_M$ bounds will be performed in the near future.

Figure 7 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 comparative purposes, the D^*_{31} coefficient in the collisionless limit from 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 the particles with the same energy $E = 100eV$ (at $B_0 = 3$ T, major radius 5.5 m) but with different atomic masses ($A = 0.2; 2; 20$). The artificial atomic masses $A = 0.2; 20$ were used only as a test for the simulations.

It is clearly seen from Figure 7 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. Real ions with $A = 2$ and $E = 100eV$ have larger gyroradius and are not amenable to a local bootstrap current calculation.

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 of memory. For the very-*lmfp* regime, $\nu/V = 3 * 10^{-6}[1/m]$, the new multi-processor VENUS+δf version with 50000 particles makes 10^6 steps on 10 processors. The computation takes $\approx$ 10 hours.

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

Several successful tests and benchmarks have been performed for the tokamak JT-60 and the stellarator W7-X, including convergence studies and the dependence of the diffusion coefficient and the bootstrap current on collision frequency and poloidal angle. We have tested several ideas to deal with the known problem of lost particles with growing weights in the long-mean-free-path regime, which is especially relevant for the stellarators. The successful benchmark with the DKES results clarifies the limitation of the concept of local transport coefficients.

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 temperature profiles (scan in radius). We hope also to compare VENUS+δf with other tools and with the experimental results in tokamaks and stellarators (W7-X, LHD, NCSX) within the framework of various international collaborations.

7. ACKNOWLEDGEMENTS

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The computational results were performed on the NEC-SX5 platform at the CSCS (Manno), at the Pleiades cluster (EPFL, Switzerland) and at the RZG (Garching, FRG).

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FIGURE CAPTIONS

Fig. 1. Time history of the normalized bootstrap current for the tokamak JT-60, with effective collision frequency $\nu^* = 0.26$ for 1000 and 6000 particles.

Fig. 2. The normalized bootstrap current from the VENUS+δf code with energy convolution versus the effective collision frequency ν^* for the tokamak JT-60. The solid line corresponds to the Hinton-Hazeltine formula $j_b \approx (1 + \sqrt{\nu}_* + 1.44\nu_*))^{-1}$.

Fig. 3. The particle flux Γ from the VENUS+δf code with energy convolution versus ν^* for the tokamak JT-60. The solid line is the analytical neoclassical result.

Fig. 4. The normalized poloidal variation of $\delta f(\theta)/f_M$ in the collisional regime with 3200, 32000 and 320000 particles in comparison with the analytical neoclassical theory.

Fig. 5. The poloidal variation of the normalized local (not poloidally averaged) tokamak bootstrap current distribution for $\nu^* = 0.065$ demonstrates the equivalence of the local approach results ("no radial drifts" with 600, 1200 and 1500 particles) and the full trajectory runs with 600 and 1200 particles.

Fig. 6. Time history of the normalized bootstrap current coefficient D^*_{31} for the inverse mean free path $\nu/V = 10^{-4}[1/m]$ with the VENUS+δf code for 1000 and 10000 particles with 10^6 time steps in the stellarator W7-X. The DKES code result is shown as the upper level, the Shaing-Callen analytic result is shown as the lower curve.

Fig. 7. The normalized bootstrap current coefficient D^*_{31} versus the inverse mean free path ν/V with the VENUS+δf code for the stellarator W7-X with atomic mass $A = 0.2$ (squares), $A = 2$ (circles), $A = 20$ (rhomboids). The Shaing-Callen analytic result is shown as the lower dashed curve. The DKES code results are shown as the upper solid curve.

Figure 1

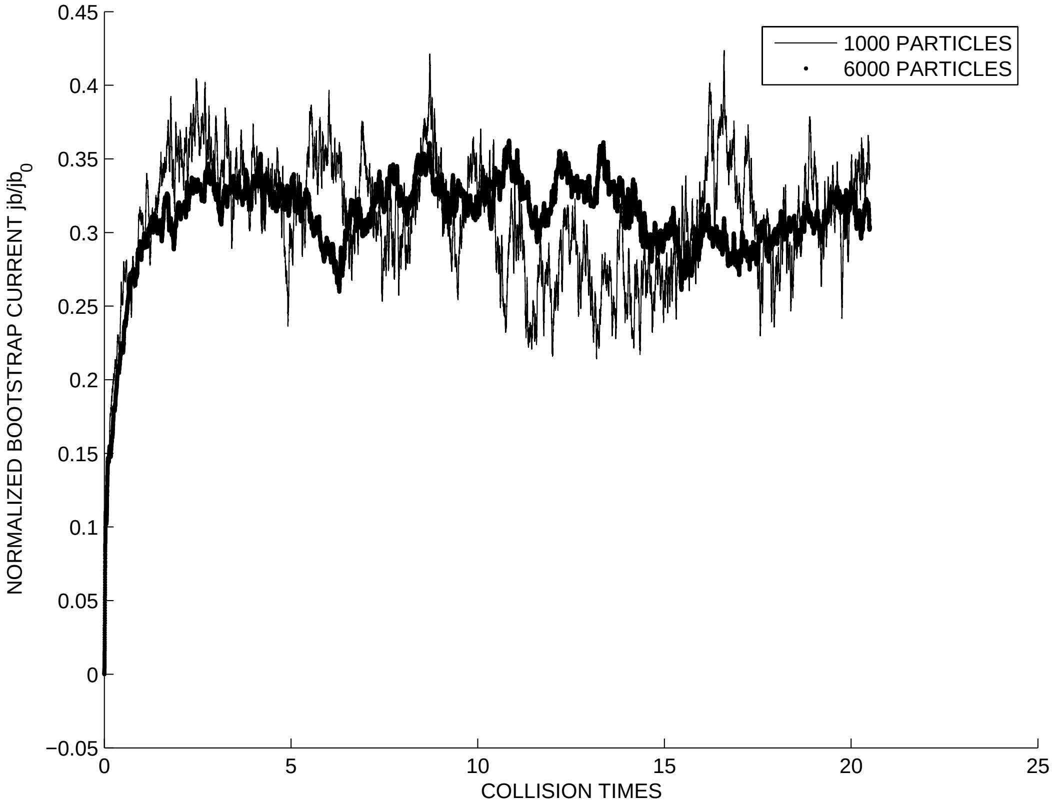
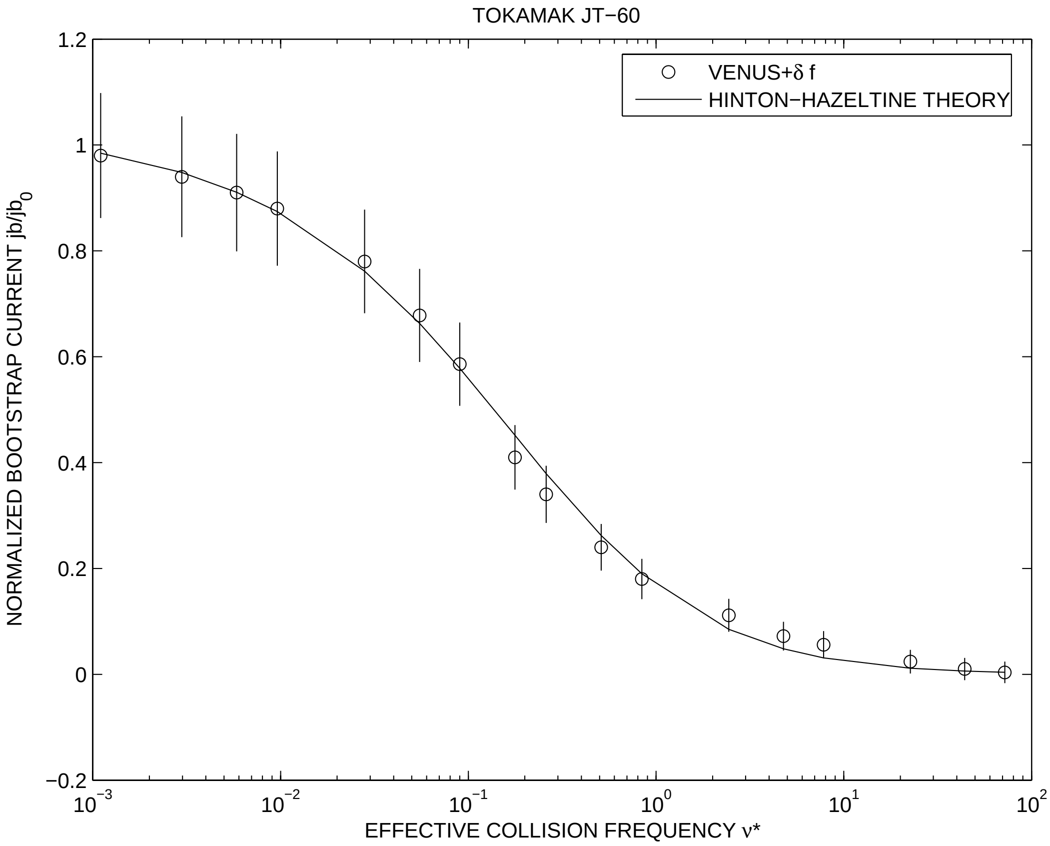
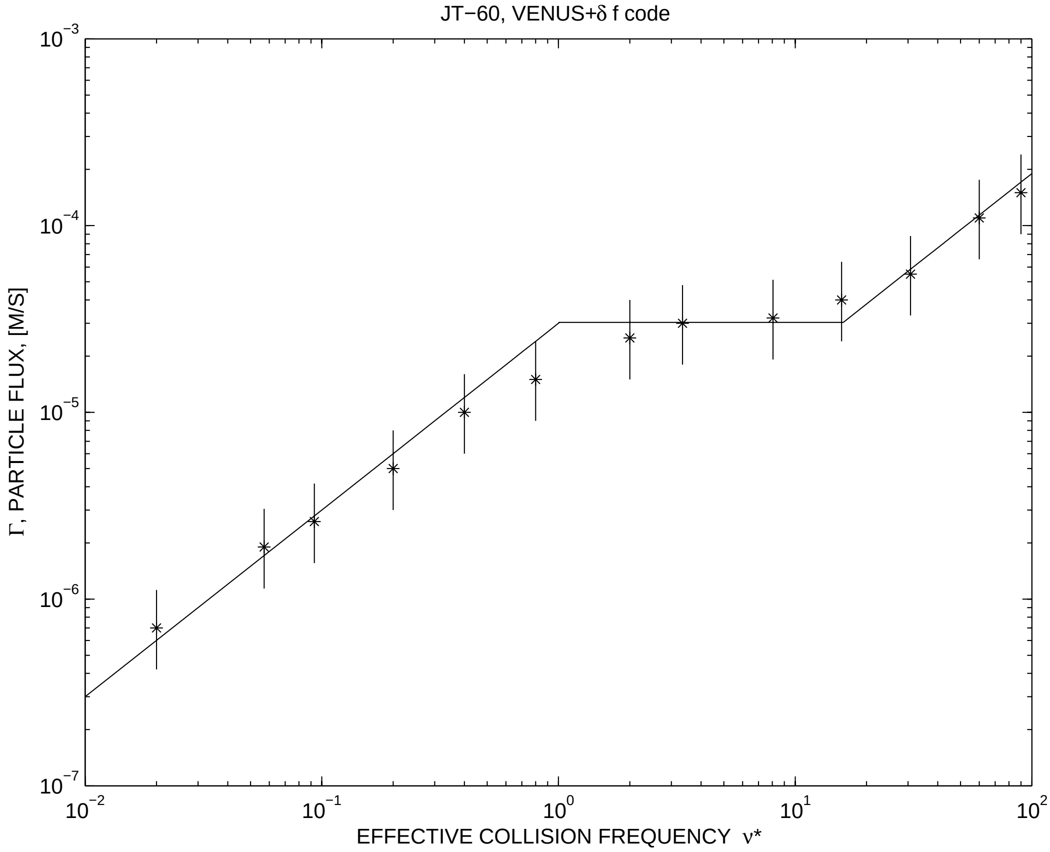

0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−0.05
NORMALIZED BOOTSTRAP CURRENT jb/jb0
1000 PARTICLES
6000 PARTICLES
0
5
10
15
20
25
COLLISION TIMES

Figure 2



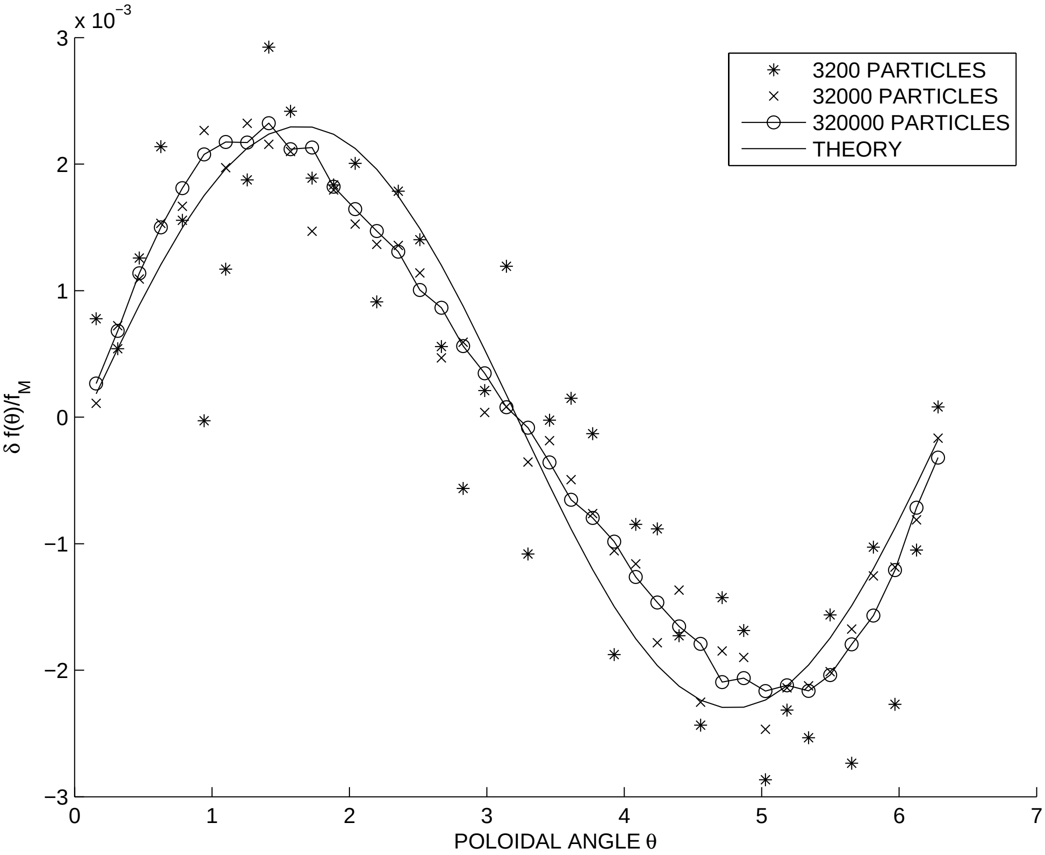
TOKAMAK JT−60
VENUS+δ f
HINTON−HAZELTINE THEORY
NORMALIZED BOOTSTRAP CURRENT jb/jb0
EFFECTIVE COLLISION FREQUENCY ν*
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
10−3
10−2
10−1
100
101
102

Figure 3



JT−60, VENUS+δ f code
10−3
10−4
10−5
10−6
10−7
Γ, PARTICLE FLUX, [M/S]
10−2
10−1
100
101
102
EFFECTIVE COLLISION FREQUENCY ν*

Figure 4



x 10^−3
3
2
1
0
−1
−2
−3
δ f(θ)/f_M
0
1
2
3
4
5
6
7
POLOIDAL ANGLE θ
3200 PARTICLES
32000 PARTICLES
320000 PARTICLES
THEORY

Figure 5

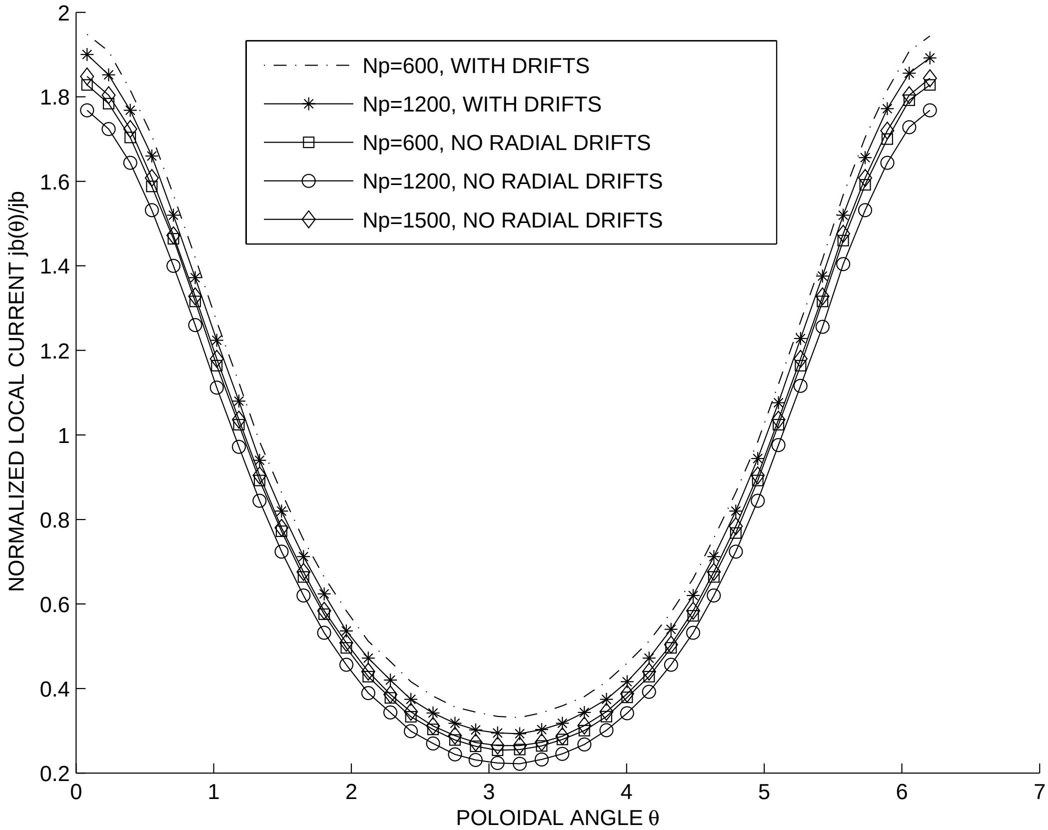

Np=600, WITH DRIFTS
Np=1200, WITH DRIFTS
Np=600, NO RADIAL DRIFTS
Np=1200, NO RADIAL DRIFTS
Np=1500, NO RADIAL DRIFTS
NORMALIZED LOCAL CURRENT jb(θ)/jb
POLOIDAL ANGLE θ
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
1
2
3
4
5
6
7

Figure 6

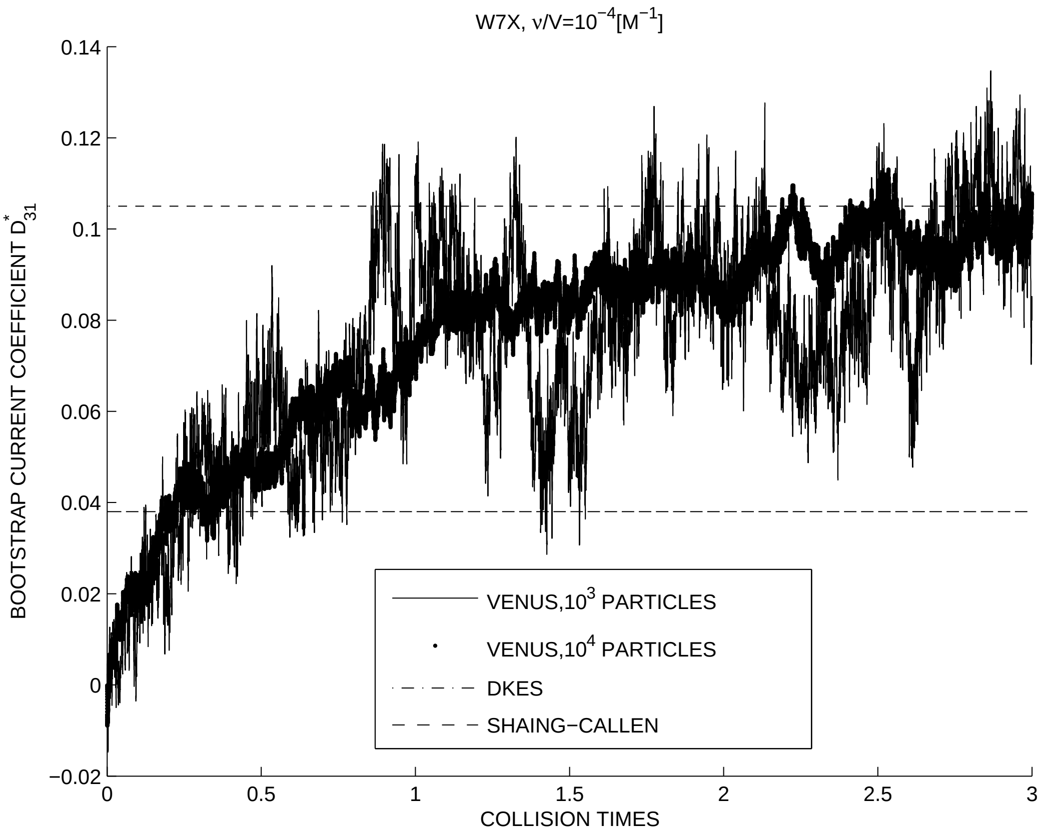
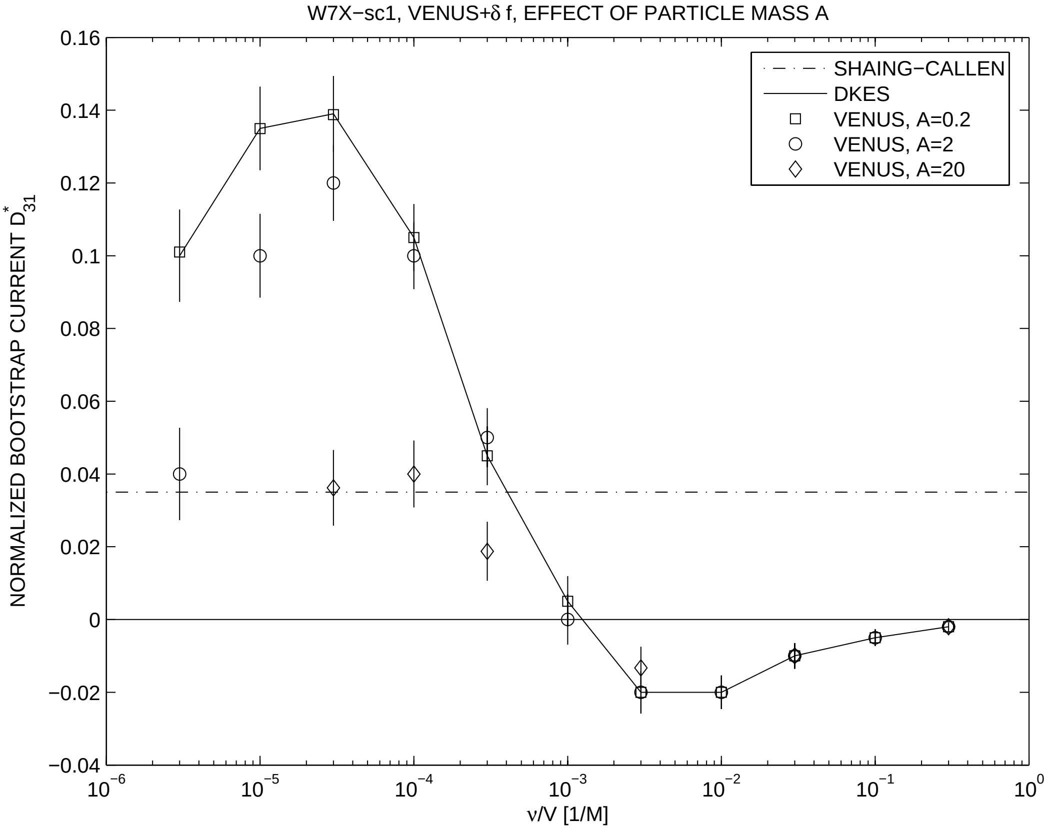

W7X, ν/V=10^{-4}[M^{-1}]
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
−0.02
BOOTSTRAP CURRENT COEFFICIENT D^*_{31}
0
0.5
1
1.5
2
2.5
3
COLLISION TIMES
VENUS,10^3 PARTICLES
VENUS,10^4 PARTICLES
DKES
SHAING−CALLEN

Figure 7


W7X−sc1, VENUS+δ f, EFFECT OF PARTICLE MASS A
NORMALIZED BOOTSTRAP CURRENT D*31
ν/V [1/M]
SHAING−CALLEN
DKES
VENUS, A=0.2
VENUS, A=2
VENUS, A=20
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
−0.02
−0.04
10−6
10−5
10−4
10−3
10−2
10−1
100