Gyrokinetic Full *f* Modelling of Plasma Turbulence in Tokamaks

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Abstract: Understanding turbulence in fusion plasmas has become a crucial task in order to achieve sufficient confinement level in large-scale devices like ITER. The ELMFIRE full *f* nonlinear gyrokinetic simulation code has been developed for calculation of plasma evolution and dynamics of turbulence in tokamak geometry. Code ELMFIRE is based on a particle-in-cell algorithm with direct implicit treatment of ion polarization and consideration of either kinetic or adiabatic electrons, and also impurities. The gyrokinetic model performs averages over the gyro-orbits while keeping accuracy over the most interesting time and length-scales regarding turbulence development. Opposite to delta *f* algorithms, the full *f* method is suitable for calculating also strongly perturbed plasmas including wide orbit effects, steep gradients and rapid dynamic changes.

ELMFIRE is here been tested against the neoclassical theory, and used for computation of the neoclassical radial electric field and the influence of turbulence on that magnitude.

1 Introduction

Plasma turbulence is a main process in the production of anomalous radial transport observed in tokamaks, that result in unacceptable loss of confinement properties. The study of turbulence and associated small scale instabilities is therefore a key issue for the understanding confinement behaviour. The features of plasma dynamics, whose particle distribution function (PDF) typically deviates from Maxwellian, require a kinetic model for its calculation, with resolution also in particle velocity space. Kinetic calculations are extremely heavy due to the number independer variables. In order to simplify the calculations, the gyrokinetic model [1, 2, 3] was introduced to reduce the dimensionality of the problem by averaging on the gyration of plasma charged particles around the magnetic field. That discards processes with frequency of the order or higher of cyclotron gyration, while keeping accuracy to the most interesting, and lower frequency, plasma processes. Gyrokinetics has become a standard tool for plasma dynamics calculation.

Gyrokinetic model has been developed following two main lines, regarding the way of describing the PDF: the full *f* and delta *f* methods. Using the delta *f* model the simulation calculates accurately only perturbations of the PDF from a given background profile, usually Maxwellian in velocity. On the other hand, using full *f* method the whole distribution function is calculated, with accuracy to arbitrarily perturbed functions always within the gyrokinetic mentioned restrictions. Using full *f* method allows for calculation of plasma dynamics in strong transients or gradients, which may induce in the PDF important deviations from the initial profiles.

There are several cases of strong transients of great importance to the study of confinement properties. The formation of Internal Transport Barrier in the plasma core, or the production of Edge Localized Modes in the plasma border. In those cases there is a rapid restructuration of both PDF and electromagnetic field. The radial electric field (E_r) and its behaviour during both equilibrium and transients is a representative magnitude for the study of confinement. Standard

neoclassical theory [7] has been tested against experiments and used as reference despite of its limitations of narrow orbits. Although effort has been made to extend its applicability [8], numerical simulations are needed for the general case of self consistent plasma-field dynamics. Computational results have been published using the delta *f* method [9], showing good agreement with the neoclassical theory even for steep gradients within the limits of the delta *f* method for the case of tokamaks, or in [10] for sterallators. Further analysis has been made [11], also using a delta *f* code, on the role of E_r on the linear and nonlinear evolution of plasma instabilities.

ELMFIRE is a full *f* global gyrokinetic code, based on a Monte Carlo algorithm and successfully benchmarked against both neoclassical theory and other gyrokinetic codes [4]. Its full *f* algorithm allows for accurate calculation in the presence of steep gradient including wide orbit effects. The first full *f* particle simulations of the evolution and equilibrium of neoclassical flows were calculated using ELMFIRE and presented in [5, 6]. That work introduced the method of one-dimensional ion polarization equation for solving the flux-surface averaged E_r.

The bulk of the article is structured in the following sections. The main features of ELMFIRE are shortly presented in section 2, giving an overwiev of its calculation methods. In section 3 is found a study of neoclassical flows and comparisons of analytical theory and simulation results. Finally are the conclusions about this work.

2 The ELMFIRE code

The code ELMFIRE solves the gyrokinetic full *f* equations for quasi-neutrality with a stochastic PIC algorithm based on Sosenko's theory of quasi particles [12]. The gyrokinetic Poisson equation is therefore written in the form

$$\nabla^2\Phi + \frac{q^2}{mB\varepsilon_0}\int\left[(\Phi - \langle\Phi\rangle)\frac{\partial\langle f\rangle}{\partial\mu} + \frac{m}{q\Omega}\langle f\rangle\nabla_\perp^2\langle\Phi\rangle\right]\mathrm{d}\mathbf{v} = -\frac{1}{\varepsilon_0}(q\bar{n_i}(\vec{r}) - en_e(\vec{r})) \qquad (1)$$

which differs from the original Lee's method of reference [2] in that the polarization drift is taken into account in the ion density while in more common approaches it is separated from the change in ion density and introduced explicitly to the Poisson equation. Here, $\Phi(\mathbf{x})$ is the electrostatic potential at the position $\mathbf{x}$, $\langle f\rangle$ is the distribution function of ion guiding centers, $\mu = v_\perp^2/2B$ is the magnetic moment, $v_\perp$ the ion perpendicular velocity component, $d\mathbf{v}$ denotes the velocity phase space differential, q, m are the ion charge and the mass, respectively, Ω is the ion Larmor frequency, $\mathbf{B} = B\hat{\mathbf{b}}$ is the magnetic field with the unit vector $\hat{b}$, n_e is electron density and the ion density $\bar{n_i}$ is obtained from the gyroaverage around the ion guiding-center coordinates which are advanced with the polarization drift included. The gyroaverage over the ion Larmor rotation is denoted by $\langle\cdot\rangle$. In the partial derivative with respect to μ the guiding-center coordinate and the parallel velocity are kept fixed.

In order to solve equation (1) one needs either to assume some average ion distribution $\langle f\rangle$, or, as in reference [13], construct it from the full *f* particle simulation together with the solution of the gyrokinetic equation for the potential Φ. Here, moreover, we use the method presented in reference [14], where the polarization drift $\mathbf{v}_p = (1/\Omega B)d\langle\mathbf{E}\rangle/dt$ is implemented directly in the guiding-center equations giving us a true average particle motion and proper diagnostics of particle transport. Here, $\mathbf{E}$ is the electric field. This equation is valid at least to order $(k_\perp\rho_i)^2$, depending on implementation, and determines the accuracy of the present method in the $k_\perp$-spectrum. Here, ρ_i is ion Larmor radius and $k_\perp$ the poloidal wave vector. In this method

the perturbation in ion density $\bar{n_i}$ by $\mathbf{v}_p$ is directly calculated from the particle orbits during simulation. This direct calculation is made implicit in $\mathbf{E}$ by evaluating the change in the ion polarization density $\delta\bar{n_p}$ at each time step by ion polarization shift using unknown $\mathbf{E}$ at the end of the time step as explained in reference [14]. For electrons, finite Larmor radius effects are neglected so that no polarization drift is applied for them.

In the simulation, the particles are initialized according to assumed density and temperature profiles and, typically, Maxwellian velocity distribution is initialized for the particle ensemble. A zero initial potential is often assumed. The so called quiescent initialization [6] of ions on numerically pre-evaluated collisionless orbits is adopted. This method is used in order to reduce the initial radial currents caused by improper poloidal distribution of particles.

After initialization, ions are advanced with a gyrophase-averaged electrostatic potential and electrons are under the influence of a bare potential in torus with circular poloidal cross section with no Shafranov shift. The guiding-center motion involves $\mathbf{E}\times\mathbf{B}$, gradient and curvature drifts, collisions and polarization drifts.

Two different coordinate systems are used: Orbits are followed in straight-field-line coordinates [15] and potential is solved in quasi-ballooning coordinates [16]. This is to avoid poor resolution in solving potential structures in straight-field-line coordinates and problems with periodicity condition in ballooning coordinates. Grid is needed only in quasi-ballooning coordinates where the potential is solved and sampling is performed. In radial direction, boundary conditions are set as explained in reference [6] with prompt reinitialization at outer boundary or, in more realistic simulations, pairwise reinitialization of outflowing ions and electrons according to assumed neutral distribution or ionization on randomly directed straight return paths of recycled neutrals can be chosen to maintain the otherwise flattening density profile.

3 Comparisons of radial electric field to neoclassical theory

Despite of the complex geometry and profiles found in real tokamak systems, it is often observed that neoclassical theory can predict, though locally, values for the heat flux. It is important that the used models for plasma simulations have consistency with the neoclassical theory, taking always into consideration that it is a simplified model that do not account all the particularities of tokamaks.

The neoclassical study performed with ELMFIRE starts with analysis of collisionless cases and relaxation process after initial transient. The geodesic acoustic modes (GAM) are present in a system initialized with a structure out of neoclassical equilibrium. Runs were scheduled using parameters from FT-2 tokamak [17] and using kinetic electron model.

As a basic comparison to theory, a set of runs were scheduled for comparing the obtained GAM frequencies (w_{gam}) and Rosenbluth residuals (A_R). The runs used homogeneous plasma with different levels of temperature ($90-360$ eV), magnetic field ($0.6-2.45$ T), major radius ($R=0.3-0.9$ m) and safety factor ($q_s=1.28-2.91$). Density was fixed to an homogeneous value of 5.1×10^{19} m^{-3}. The charge current profile was selected for constant q_s over the simulated region. In figure 1 are shown the results, both for GAM frequencies and Rosenbluth residual, plotted against the predicted values following the neoclassical expressions:

$$w_{\mathrm{gam}}=\frac{v_{Ti}}{R}\sqrt{\frac{7}{4}+\frac{T_e}{T_i}} \qquad A_R=\left(1+\frac{1.6q_s}{\sqrt{r/R}}\right)^{-1} \tag{2}$$

A fair agreement has been found with the analytical values, despite of the effects arising

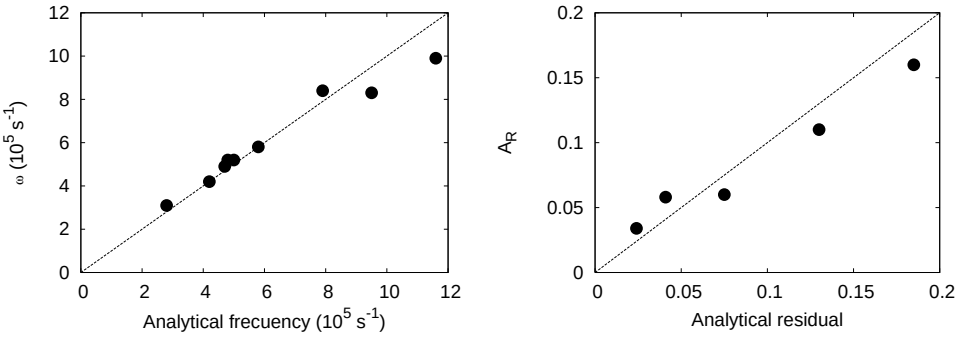

Figure 1: Comparison of GAM frequencies (left) and Rosenbluth residual (right), against analytical values predicted by neoclassical theory.

from boundaries, since the GAM theory has been developed for periodic system with adiabatic electrons. The Landau collisionless damping was found higher than the theory predictions, in part due to the use of kinetic electrons and to the influence of boundaries. It is the global nature of the code what makes more difficult the analysis of infinite and homogeneous systems like in this case.

Special analysis was made to study the time evolution of E_r under different configurations. Previously flux-surface averaged full f simulations of ELMFIRE have given the neoclassical (Hazeltine-Hinton, HH) radial electric field when parameters have been appropriate for the analytical expressions [18], which has been investigated for different polarization models. However, when a non-averaged gyrokinetic field model is adopted, the effects of turbulence and neoclassical physics become inseparable, with turbulent fluctuations and flows affecting neoclassical physics and vice versa.

To investigate the coupled dynamics of neoclassical and turbulent transport, geometrical and profile parameters were loosely adopted from FT-2 tokamak, with major radius $R_0 = 0.55\,\mathrm{m}$, minor radius $a = 0.08\,\mathrm{m}$, toroidal magnetic field $B_T = 2.2\,\mathrm{T}$, total plasma current $I = 55\,\mathrm{kA}$ and a current density profile of $j(r) = j_0(1-(r/a)^2)$, simulation region of $r/a = 0.25-0.5$, density and temperature profiles as given in figure 2, with deuterium as the only ion species. In the following discussion we use the following definitions: $v_t = \sqrt{2\,k_B T_i/m_i}$, $\rho_i = v_t/\Omega$ with $\Omega = q_i B_T/m_i$ with ion charge q_i, mass m_i, k_B is the Boltzmann constant, $\rho_{par} = v_t/\Omega_p$ with $\Omega_p = q_i B_p/m_i$ and B_p is the poloidal component of the magnetic field, $\varepsilon = r/R_0$ is the local inverse aspect ratio and r the local radial coordinate. In the simulation the $n_{e,i}$ and $T_{e,i}$ profiles were allowed to relax, however heat was slowly removed from the outer boundary with escaping particles on the outer edge reinitialized according to a preset cold neutral profile. Boundary conditions for the field equations were set as follows: on the inner boundary potential was taken to zero, and on the outer boundary the radial component of the electric field was allowed to vanish. The finite differencing grid in the simulation is $31 \times 200 \times 4$ in radial, poloidal and toroidal directions respectively in field-aligned coordinates. The time step is $\Delta t = 50\,\mathrm{ns}$.

In the results, the turbulent fluxes have reached a dynamical saturated state after $50\,\mu\mathrm{s}$. After initial transient of the heat flux, due to the linear growth of modes and decay of initialization values, the radial electric field reaches the value predicted by the neoclassical theory on the middle region of the simulation ($r/a = 0.6125$), as shown in figure 3 left. The calculated oscillations near the outer boundary correspond to a GAM oscillation. The ion heat conductivities normalized to $\chi_{GB} = \rho_i^2 v_{ti}/2a$ are shown in figure 3 right.

Neoclassical theory (in terms of the Hazeltine-Hinton field) has been observed to break

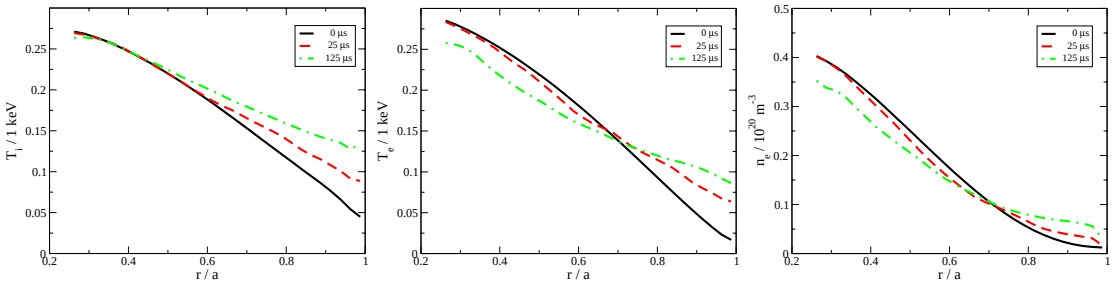

Figure 2: Radial temperature profiles for electrons (T_e) and ions (T_e), and density profile for electrons at simulation times of 0 μs, 25 μs, and 125 μs. Initial temperature for ions and electrons are the same.

down when Mach numbers are large, and when ρ_{pol}/L_T is large enough [18]. Based on figure 4, we would expect the best agreement to HH field to occur at the region of $r/a = 0.75$. However, in the simulation this is also where the modes grow strongest. The fluctuations may thus inhibit the neoclassical radial electric field through non-ambipolar fluxes from finite Larmor radius effects.

As given by Stringer in [19, 20], finite Larmor radius effects in the presence of fluctuations may drive non-ambipolar neoclassical transport. The radial current thus driven may be given, as a rough estimate, in the limit of small representative wavenumber k as $j_{E\times B} = \rho_i^2 k^2 \Gamma_e/4$, where the electron charge flux Γ_e is assumed to arise only from $E \times B$ drift motion, and the Mach number M_p is assumed to be small. Assuming that the neoclassical current and electric field contributions cancel with temperature and density gradient terms, we may approximate the neoclassical current balance for fluctuations as

$$j_{E\times B} = -\frac{q_i n_i D_i}{T} E_r' \tag{3}$$

where $D_i = \sqrt{\pi}/2\varepsilon^2 \frac{T}{\Omega B_p} \frac{\nu_t}{r}$ in the plateau regime. From the turbulence spectra in the saturation state we obtain $k\rho_i = 0.25$, whence we may solve the neoclassical current balance for fluctuations. It is important to note, that the contribution E_r' from fluctuations would be added to the neoclassical field, and thus the fluctuations may suppress the neoclassical electric field. Also, the same contributions would arise from numerical particle noise, and as such, figure 5 puts an upper limit to noise contributions.

The contributions from fluctuations appear to be insignificant (especially where better agreement with neoclassical theory would be expected), and as such, warrants a different interpretation: the turbulence may drive also Reynolds stresses (see reference [21]). To assess what mechanism lies behind the difference observed in figure 3, we show also the flux surface averaged and time-integrated $R_{r\theta} = \int_{t_0}^{t} -\partial_r \{v_r v_\theta\}\, dt'$ component of Reynolds stress in figure 5. As the poloidal rotation evolution is influenced by Reynolds stress (which acts as torque), the time-integrated Reynolds stress corresponds to rotation velocity, and as a negative radial electric field produces rotation in the positive direction, we may assert that a positive time-integrated Reynolds stress corresponds to negative E_r and vice versa. The time integrated Reynolds stress profile does indeed fit very well with the observations of the disagreement with HH field, as the stress peaks near the points where differences are observed, whereas in the flat region of Reynolds stress we observe a satisfactory agreement with neoclassical estimates.

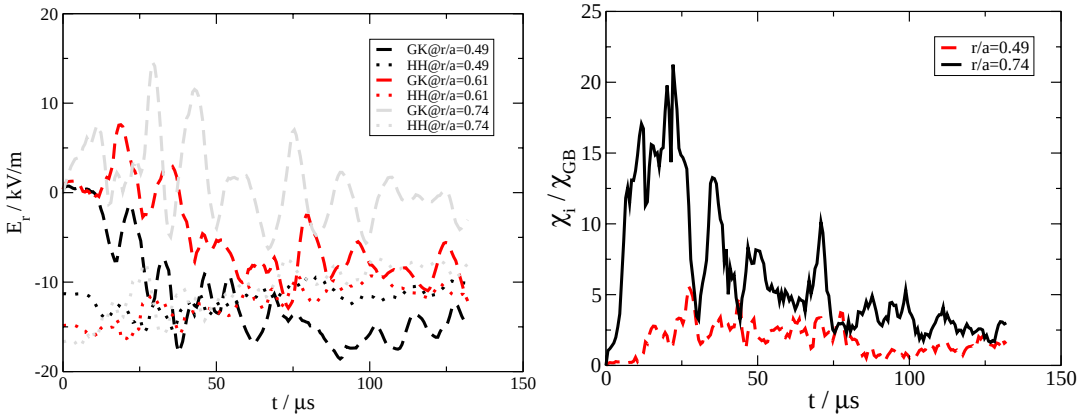

Figure 3: Comparison of flux surface averaged E_r, on three radii of the simulation region (r/a is 0.49, 0.61 and 0.74), with the corresponding Hazeltine-Hinton model predictions (left). To illustrate the evolution of turbulence, the ion heat conductivity χ_i is shown (right).

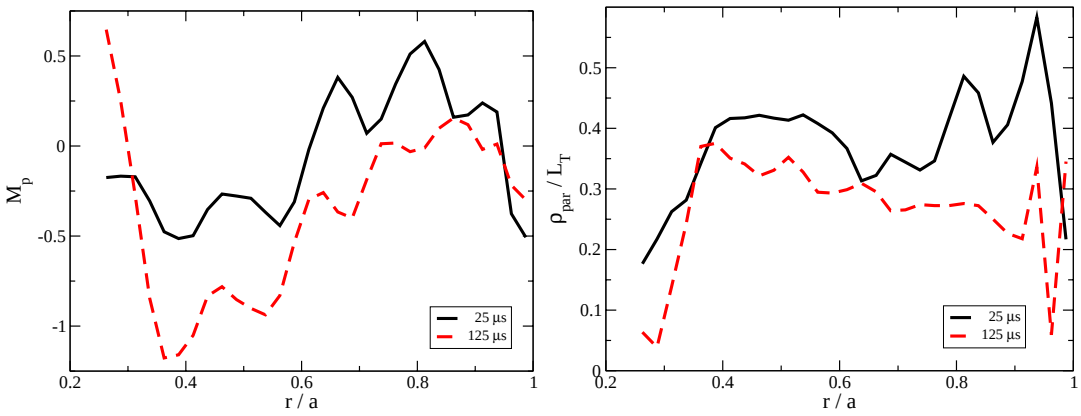

Figure 4: The poloidal Mach number ($E_r/B_p v_t$) promptly after saturation of ion heat flux and near the end of the simulation (left), and banana widths normalized to temperature gradient scale length (right).

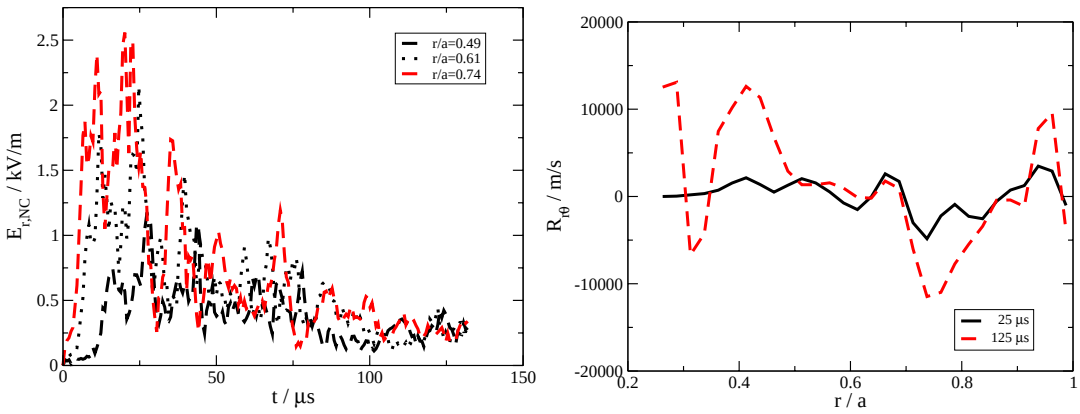

Figure 5: Neoclassical radial current from equation (3) during the simulation, and the Reynolds stress as obtained from the PDF.

4 Conclusions

A full *f* gyrokinetic global particle code named ELMFIRE has been developed and tested against neoclassical theory. The code includes direct implicit ion polarization and either kinetic or adiabatic model for electrons. The comparisons show good agreement for GAM frequencies, Rosenbluth residual and radial electric field, where applicable. The obtained results are very positive, as many characteristics of the neoclassical theory have been reproduced, even in the presence of a moderate level of turbulence. Based on the current simulations, Reynolds stress contributions from turbulence mediate the evolution of neoclassical fields.

Acknowledgements

This project has received funding from the European Commission. The facilities of the Finnish IT Center for Science have been used for this work.

References

[1] TAYLOR, J.B., HASTIE, R.J., "Stability of general plasma equilibria - I formal theory", Plasma Phys **10** (1968) 479.

[2] LEE, W.W., "Gyrokinetic approach in particle simulation", Phys Fluids, **26**, (1983) 556.

[3] DUBIN, D.H.E., et al., "Nonlinear gyrokinetic equations", Phys Fluids, **26**, (1983) 3524.

[4] HEIKKINEN, J.A., et al., "Gyrokinetic simulation of particle and heat transport in the presence of wide orbits and strong profile variations in the edge plasma", Contrib. Plasma Phys. **46**/7-9 (2006) 490.

[5] HEIKKINEN, J.A., et al., "Neoclassical Radial Current Balance in Tokamaks and Transition to the H Mode", Physical Rev. Lett. **84** 487 (2000).

[6] HEIKKINEN, J.A., et al., "Particle Simulation of the Neoclassical Plasmas", Journal of Computational Physics **173** (2001) 527.

[7] HINTON, F.L., HAZELTINE, R.D., "Theory of plasma transport in toroidal confinement systems", Rev. Mod. Phys. **48** (1976) 239.

[8] LIN, Z., et al., "Neoclassical Transport in Enhanced Connement Toroidal Plasmas", Phys. Rev. Lett. **78** (1997) 456.

[9] WANG, W.X., et al., "Neoclassical radial electric field ans transport with finite orbits", Phys. Rev. Lett. **87** (2001) 055002-1.

[10] LEWANDOWSKI, J.L.V., et al., "Gyrokinetic calculations of the neoclassical radial electric eld in stellarator plasmas", Phys. Plasmas **8**/6 (2001) 2849.

[11] ALLFREY, S.J., et al., "The role of radial electric fields in linear and nonlinear gyrokinetic full radius simulations", New Journal of Physics **4** (2002) 29.1.

[12] SOSENKO, P.P., et al., "Krylov-Boholiubov Methods and Gyrokinetics", Physica Scripta **64** (2001) 264.

[13] HEIKKINEN, J.A., et al., "Full f particle simulation method for solution of transient edge phenomena", Contrib. Plasma Phys. **44** (13) 2004.

[14] HEIKKINEN, J.A., et al., "Gyrokinetic simulation of neoclassical and turbulent transport", 31th EPS Conference on Plasma Physics and Controlled Fusion (2004) P-5.161.

[15] WHITE, R.B., et al., “Hamiltonian guiding center drift orbit calculation for plasmas of arbitrary cross section”, Physics of Fluids **27** (1984) 2455.

[16] DIMITS, A.M., “Fluid simulations of tokamak turbulence in quasiballooning coordinates”, Phys Rev. E **48** (1993) 4070.

[17] LASHKUL, S.I., et al., “ Effect of the radial electric field on lower hybrid plasma heating in the FT-2 tokamak” Plasma Phys. Rep. **27** (2001) 1001.

[18] KIVINIEMI, T.P., et al., “Neoclassical radial electric field and ion heat flux in the presence of the transport barrier”, Contrib. to Plasma Phys. **42**/2-4 (2002) 236.

[19] STRINGER, T.E, “Non-ambipolar neoclassical transport”, Nuclear Fusion **35**/8 (1995) 1008.

[20] STRINGER T.E., “Neoclassical transport in the presence of fluctuations”, Nuclear Fusion **32**/8 (1992) 1421.

[21] NAULIN, V., “Aspects of flow generation and saturation in drift-wave turbulence”, New Journ. of Phys. **4** (2002) 28.1.