Full f Gyrokinetic Simulation of Tokamak Plasma Turbulence Using ELMFIRE

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Abstract. Gyrokinetic particle-in-cell simulation on a transport and microinstability time scale is performed with the ELMFIRE code for a small tokamak FT-2 with kinetic electrons. Turbulent modes are characterized based on their poloidal phase velocity, and tentative comparison with the Doppler reflectometric measurement is done for the poloidal mode rotation. Cyclone base case comparison with adiabatic electrons reveals the need for a sophisticated adiabaticity model in the presence of finite ion orbits. Progress in the simulation of the edge pedestal in L-H transition conditions for a medium-sized tokamak is reported.

1. Introduction

Large-scale kinetic simulations of toroidal plasmas based on first principles are called for in studies of such transient transport mechanisms like Low (L) to High (H) confinement barrier formation or Edge Localized Modes (ELM) at the edge plasma, Internal Transport Barrier (ITB) formation in the core plasma, or intermittent turbulence in magnetic fusion devices. Because of rapid or strong restructuring in the particle distribution function f(**x**,**v**,t) and in the EM field, accompanying such transients, full f kinetic calculation is a necessity in such cases.

ELMFIRE [1] is a global gyrokinetic full f particle-in-cell code designed for first principles transport simulation in tokamaks including both neoclassical and turbulent physics. It is based on an implicit gyrokinetic model and a set of guiding-centre equations, field equations, and energy conservation law derived with Lie perturbation method from an appropriate Lagrangian. The guiding-centre motion includes polarization drift, and the coefficient matrix of the Maxwell equations is straightforwardly updated from the simulated f(**x**,**v**,t). Presently, the code is electrostatic with small-amplitude fluctuations having frequencies $\omega << \Omega_i$, where Ω_i is the ion cyclotron frequency. The parallel acceleration of electrons by the electric field is treated implicitly for stability.

2. Validation and benchmarking

The Cyclone Base case has become a standard benchmark case for tokamak plasma turbulence simulations. The case has also been adopted as the standard transport benchmark for the EFDA task-force ITM turbulence project [2]. Several Cyclone Base benchmarks (e.g., linear growth rates) have been obtained [1] with ELMFIRE. In full f global nonlinear simulation with adiabatic electrons it is found that the adiabatic condition has to be modified to correctly evaluate finite ion orbit effects on electrostatic potential with temperature and density profile variations of the plasma.

Fig.1 shows the ion heat conductivity as a function of time at the mid-radius position of the Cyclone base case with adiabatic electrons. The adiabaticity for the electrons is defined as

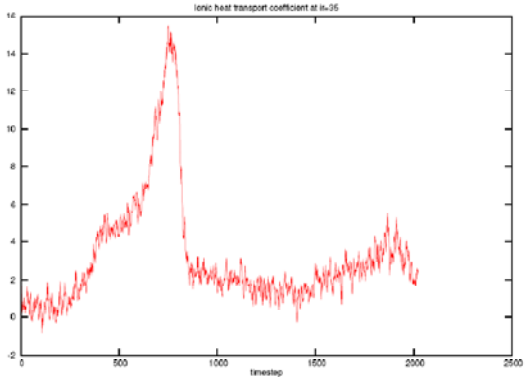

Fig.1 Ion heat transport coefficient (in m^2/s) as a function of time for the mid-radius position in the Cyclone Base case.

usual with the formula $n_e = n_0(r)\left[1 + e(\Phi - \langle\Phi\rangle / kT(r)\right]$, where Φ is the electrostatic potential and n_e is the electron density at the same position. $\langle\Phi\rangle$ is the flux-surface averaged potential. This assumption fixes the radial density profile to $n_0(r)$ due to quasineutrality condition. It is of interest to note that the ion heat diffusivity saturates at fairly low value (much less than the gyro-Bohm value) after the initial overshoot due to the linear growth phase.

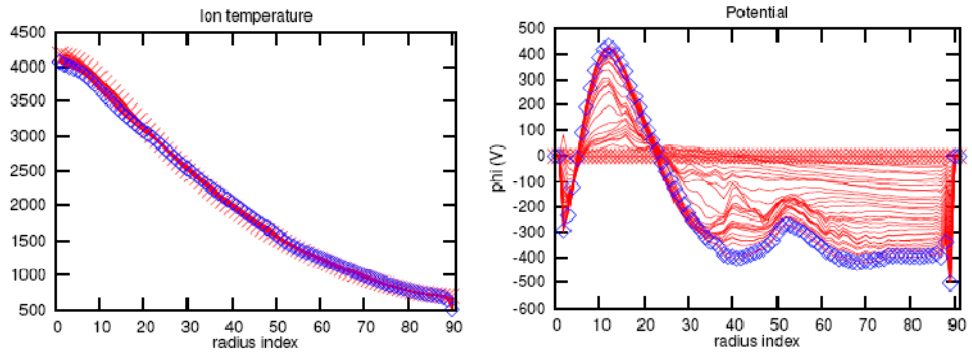

Fig.2 Evolution of flux-surface averaged radial profiles of ion temperature (in eV) at left and potential at right in the Cyclone base case for adiabatic electrons. Final values are denoted by diamonds.

In order to understand this, it is important to note from Fig.2 that the electrostatic potential becomes bipolarly perturbed by the ion temperature profile relaxation. If, for simplicity, one takes the perturbation $a\cos(r/b)$ of the ion orbit half width w due to the ion temperature relaxation along the radial direction r, the related shrinking and widening of orbits causes an ion density perturbation $-(aw/3b^2)n_0\cos(r/b)$, where n_0 is the unperturbed density at $r/b=\pi/2$. Taking into account of the ion polarization, quasineutrality condition gives the potential perturbation $-\Omega\, aB(w/3)\cos(r/b)$, where Ω is the ion cyclotron frequency and B is the magnetic field.

We calculate the amplitude $-\Omega aBw/3$ for the ELMFIRE cyclone base case simulation in Figures 1 and 2. Here, $B=1.9$ T, $\Omega = 10^8$ s^{-1}, and $w=2.5$ cm for thermal bananas at radius index 25 (the node of bipolarity $r/b=\pi/2$). The relative ion orbit width perturbation a/w can be, directly read from the data e.g., at the end of calculation: From the picture of T_i profile, we

read for the perturbation T_i about *-250* eV at the inner relaxation maximum implying *a/w=-0.035*. If these numbers, and the fraction of trapped ions *0.3*, now are put into our expression of potential perturbation amplitude, we get *500* V at the inner relaxation maximum for the potential perturbation at the end of calculation.

Note that we have a negative *a* at the radius index 10 (negative maximum of perturbation) which means a positive potential maximum at that point. Both the direction and amplitude of the resulting bipolar potential perturbation from ELMFIRE simulation are in fair agreement with this theory.

What matters here is the magnitude of T_i and its relaxation. The larger T_i or its relaxation, the larger is the effect. In our Cyclone base simulations, we have taken T_i ~4000 eV at the inner edge. T_i relaxation is also enhanced by the (unphysical) initial transient in ion heat diffusivity in simulations. Thus, for comparison of results from different codes, we have to look at whether the T_i relaxation is equally strong and T_i is at the same level (ion orbits wide enough to clearly see the effect). E.g., any effort to keep the inner edge in thermal bath with T_i fixed there in some codes may mask this effect.

When electrons are kinetic and collisions are taken into account, the above effect can appear only transiently. Collisions take care about the return ion current which neutralizes the charge separation from ion orbit modification sooner or later. Also, T_i relaxation is now also partially controlled by ambipolar electron/ion radial convection. Convective heat losses do not cause orbit modifications. In kinetic ELMFIRE simulations with collisions, we have not yet seen the effect clearly.

The result means that it is not possible to calculate saturation in the adiabatic limit in the full *f* code unless electron adiabaticity is redefined to prevent charge separation through the ion orbit shrinking/widening (but this may cause other problems) or unless T_i profile is kept unrelaxed (by some thermal bath or similar ways). In the kinetic case, collisions and electron/ion convection ultimately cancel this charge separation thus preventing any steady potential bipolarity (the latter may appear only transiently for weak collisions).

The fluctuation structures in macroscopic quantities can be studied with help of wavelets. The 2D continuous wavelet transform on a poloidal cross-section enables the extraction of specific structure sizes from the original data. Using isotropic Mexican hat and anisotropic Morlet wavelet functions in the analysis the spatial properties of fluctuation structures of a given scale can be investigated. Furthermore, the fluctuation structures under consideration can be related to a specific simulation phase, e.g. to turbulence, by controlling the threshold value. Combining the wavelet analysis and the time-evolving data we are able to trace the movement of fluctuation structures on a poloidal plane. In addition, the average development of spatial properties can be viewed and compared to the evolution of simulation phases, e.g. to the generation of ITB and H-mode.

In Fig. 3a, as an example of such analysis, the continuous wavelet transform is used to reveal the structures of large-scale density fluctuations after the linear growth has saturated in a Cyclone base case simulation. Furthermore, the time evolution of the number of large-scale density fluctuations induced by turbulence is shown in Fig. 3b. Here, the focus is in the structures, which are of the size of *7* cm.

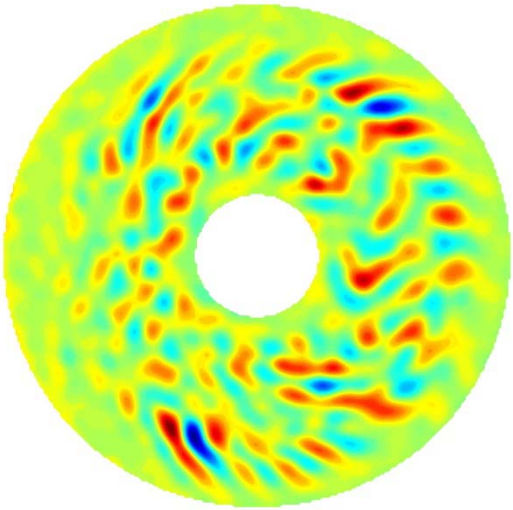

Figure 3a. The large-scale density fluctuations on a poloidal plane are revealed by using wavelet techniques.

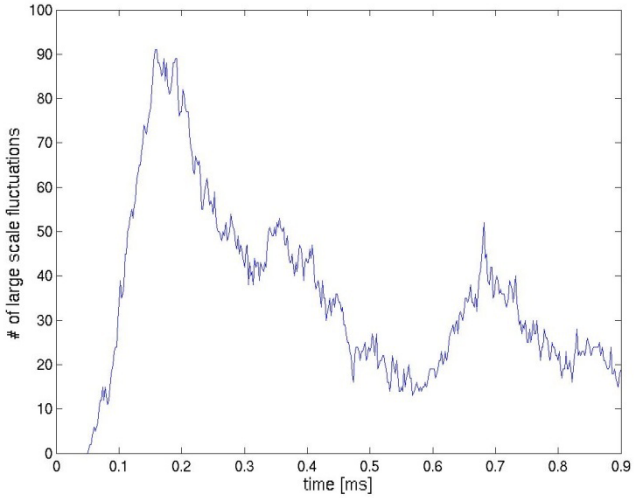

Figure 3b. Turbulence generates and sustains a considerable amount of large-scale fluctuations.

3. FT-2 transport simulations with kinetic electrons

Experimental benchmarking of the ELMFIRE code is performed in co-operation with the small FT-2 tokamak experiment at the Ioffe Institut in St Petersburg. Poloidal velocity obtained from ELMFIRE simulations is compared to experimental results from reflectometer diagnostics [3]. Doppler reflectometry measures the poloidal velocity by evaluation of the rotational velocity from the Doppler frequency shift of back scattered radiation [4] . The output signal of the microwave mixer is given by $I(t) = \int W(r,\theta)\delta n(r,\theta,t) dr d\theta$ where $W(r,\theta)$ is the complex spatial weighting function and δn(r,θ,t) the density fluctuation. The weighting function depends on the antenna and the receptivity of the waves and is obtained by a ray tracing code [4]. In our model the density fluctuations are produced by the ELMFIRE code and the microwave signal I(t) can be reproduced by multiplication and integration of the density fluctuations with the weighting function. Resent comparisons between the experimental and simulated power spectrum of I(t) show good agreements in both the shift of the spectrum as well as the width of the power spectrum. Underlying phenomena causing the poloidal velocity can now be studied with the ELMFIRE code. In figure 4, the simulated $E_r \times B$ velocity and total poloidal velocity of fluctuations, obtained from correlation studies are shown for typical Ohmic FT-2 parameters [5]. The outer and inner parts show good agreement where in the central part a difference is found. At the central region of the simulation, a contribution of trapped electron mode (TEM) phase velocity has been found from linear mode analysis, explaining the difference in figure 4. The angular frequencies and growth rates obtained from the ELMFIRE linear mode analysis have been successfully benchmarked against the eigenvalue code GS2 [6], see Figure 5. It can be concluded that for the plasma parameters given in [5] $E_r \times B$ velocity arising from neoclassical and turbulent mechanisms is the main contributor to the Doppler shift of the power spectrum of I(t) at the inner and outer region of the experiment with a medium sized contribution of the modes phase velocity of TE modes at the central region of the simulation.

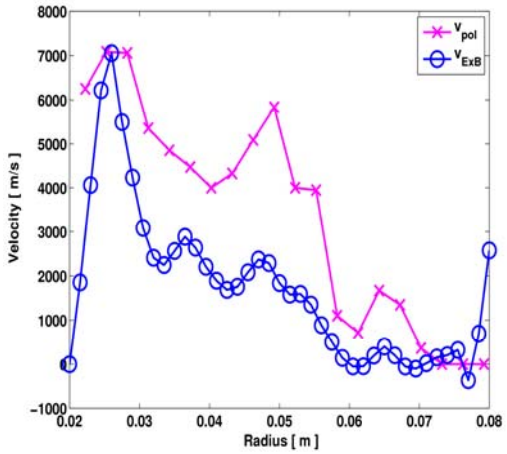

Fig 4. The simulated $E_r \times B$ velocity and total poloidal velocity of fluctuations in FT-2.

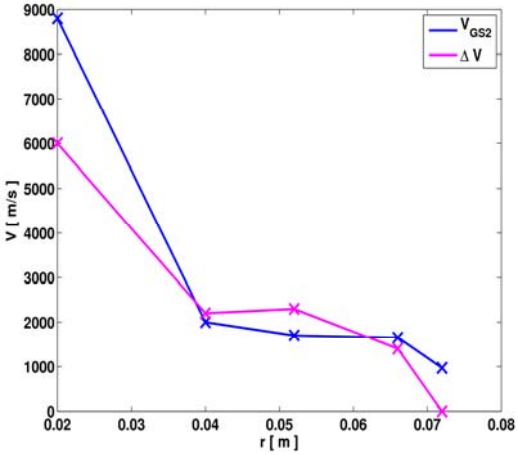

Fig.5 The ELMFIRE phase velocity (Δv) versus the phase velocity obtained with linear GS2 calculations.

4. Code scalability and memory management

The ELMFIRE code demands powerful computational resources for the typical cases under simulation. Because of the limitations of processor capacities, the code has been prepared and optimized for parallel computation. The standard for communication among processes is MPI, with special care of both memory and disk parallel operations. ELMFIRE has two key tasks that have to be taken care of when doing parallelization: the time advance of particles and the calculation of the matrix corresponding to the discretized girokinetic Poisson equation. The parallelization of particle advance, once calculated the electromagnetic field, is straightforward since at that level particles do not interact among themselves. Particles are just splitted into all available processors, which perform the calculations with perfect scaling.

However the parallelization of the calculation of the electric field, specially the construction of the discretized problem matrix, is a more complicated and has been dealt mainly using two different advanced original techniques. The first technique [7] uses AVL trees for compactly storing the sparse matrix coefficients, which are updated many times during the matrix construction. Therefore AVL is most suitable for being compact, include fast searches and easeness of parallelization. The results of the AVL implementation into ELMFIRE have shown a very good scalability regarding memory distribution, but a heavy non-collective network communication, which may lead to longer computation time.

The second implemented technique is Domain Decomposition [8], which has been programmed for toroidal decomposition of the toroidal system. This technique, as shown in the reference, produces strong memory savings at a negligible (or even favourable) computation time increase. However this technique produces limited improve in parallel scalability since the decomposition is limited to the number of toroidal cells in the system, which in straight-field coordinates is usually low. The code as it is now has achieved good scalability until the few thousand processors, but a combined implementation of both techniques would lead to a still further kick to parallel scalability until high levels ($\sim 10^4$ procs). We keep in mind that a global simulation of ITER would require this performance or even higher, which has been (and still is) leading our efforts and results towards that direction.

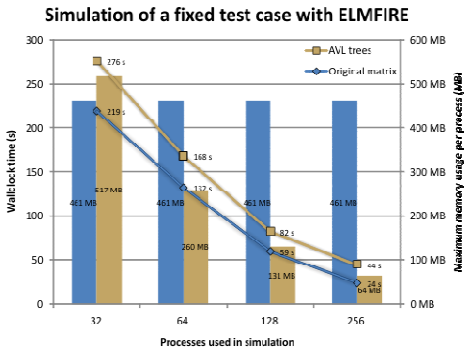

Fig.6 Scalability demonstration with data storage using AVL trees.

5. Pedestal simulations in a medium-sized tokamak

In the L-H transition, a transport barrier is created by external heating, which is considered an important part of the reactor plasma operation. In order to self-consistently simulate a transport barrier generation both neoclassical and turbulence physics as well as proper boundary conditions and heating operator are required and are included in ELMFIRE. It is also important that the numerical techniques in the code are valid in the plasma edge where the gradients are steep and distributions can much deviate from Maxwellian. In [9], such simulations were done for inner plasma of FT-2 tokamak using ELMFIRE which already was very CPU-intensive. Extending such simulation from small to medium size tokamaks is a computational challenge, but is now possible using AVL method with large-scale supercomputing facilities. After latest code optimizations ELMFIRE could be run with *500* processors for a *100x600x32* grid using *500* particles per cell, acceptable for turbulence saturation studies in reasonably sized annular volumes inside the ASDEX Upgrade toroidal plasma. In typical test runs, however, *300* million ions and electrons (~ *4000* per cell for lower noise level) are followed in a *30x600x4* grid with 10^{-7} s time steps. Such simulations run up to *0.2* ms in *48* hours with *256* processors and can be used for tentative analysis although longer simulations (*1* ms or more) are important in order to see orbit effect with more realistic parameters.

In Fig. 7a, typical example of such a simulation is shown. Here, parameters similar as in ASDEX Upgrade are used and plasma is heated strongly in a narrow regime near the inner radius (r = 42 cm) of the simulation regime by letting them collide with a fixed background which is in higher temperature than the test particles. After some 0.02 ms, heat pulse initiated from strong heating at inner edge reach the outer radii. However, in the simulations it is difficult to separate time behaviour of transport coefficients caused by the heating model from the linear growth which will occur even without heating. In Fig. 7b, only a modest poloidal rotation is observed from the correlation analysis of the density data indicating L-mode condition. This rotation is mostly explained by ExB velocity. Near the outer edge where both physics effects and numerical effects due to boundary conditions affect the results discrepancy exists. The shear in poloidal rotation is still below the threshold for strong turbulence suppression unlike observed earlier in [10] where only neoclassical effects were taken into account. However, there the simulation time was long enough to take into account the ion orbit loss mechanism. Also, as real transport time-scale simulations are not yet possible, results maybe sensitive to given initial profiles and more careful checking of the effect of numerical parameters, noise and initialization is needed.

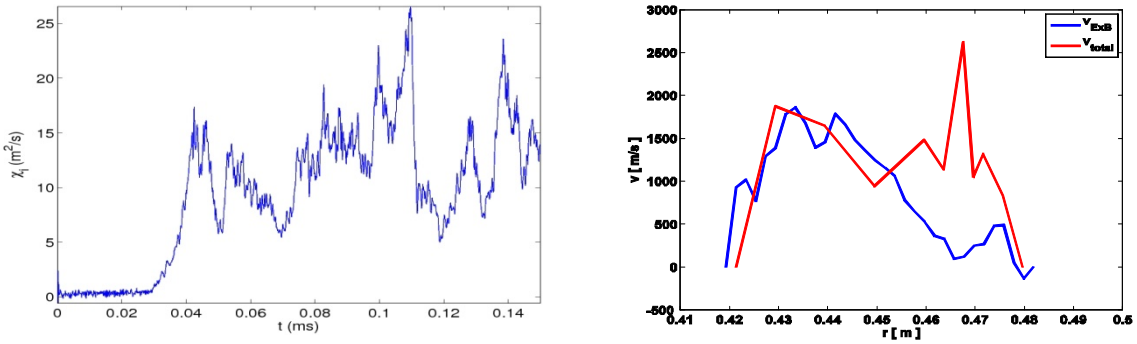

Figure 7. a) Heat transport starts to grow when heat pulse reaches outer radii (r = 46 cm). b) Modest poloidal rotation is observed from the correlation analysis of the density data for ASDEX Upgrade indicating L-mode condition. This rotation is mostly explained by ExB velocity, but near the outer edge discrepancy exists

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