Gyrokinetic total distribution simulations of drift-wave turbulence and neo-classical dynamics in tokamaks with ELMFIRE

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Abstract:

One of the outstanding problems of transport processes in tokamaks is the L-H transition and in general transport barrier formation, explanation of which has attracted several possible hypotheses ranging from purely neo-classical (rotational runaway) to non-linear (modulational) instabilities between turbulent eddies and zonal flows. Total f gyrokinetic simulation allows for the investigation of all the most important transport processes simultaneously, or by distinguishing between neo-classical and turbulent mechanisms in flow generation and transport. ELMFIRE is a gyrokinetic 5D total distribution simulation capable of transport time scale simulations of a multi-species plasma with self-consistent evolution of microturbulence, neo-classical physics and large scale structures. Generally gyrokinetic investigations of neo-classical processes have been obtained potential flux surface averaging, eliminating all modes except the $(0, 0)$ zonal mode in simulations. We present an improved model for gyrokinetic particle simulations of neo-classical physics. We also discuss theoretical aspects of the gyrokinetic theory which includes the polarization drift in particle equations of motion, and present conservation of total angular momentum and energy in ELMFIRE . The role of sampling error is investigated, and the effect of noise on long time scale evolution of the system.

1 Introduction

Thermal transport in a magnetised plasma is intimately related to the biggest unsolved physics problem of turbulence. Small scale, low frequency instabilities drive that turbulence and its study is therefore of crucial importance for improving confinement efficiency. The overall interaction of those small scale processes can however be correctly simulated with global kinetic simulations that cover all, or a significant part, of the whole tokamak. Confinement modes that suppress this micro-turbulence (such as the high confinement mode, or H-mode) have been observed, and one of the outstanding problems of transport processes in tokamaks is the L-H transition and in general transport barrier formation, explanation of which has attracted several possible hypotheses ranging from purely neo-classical (rotational runaway and orbit losses) to modulational instabilities between turbulent eddies and zonal flows, to name a few. Total f gyrokinetic simulation allows for the investigation of all these processes simultaneously. Elmfire code [1] solves the gyrokinetic full f equations for quasi-neutrality with a gyrokinetic PIC algorithm based on a variation of the gyro-kinetic model developed in Ref. [2].

The Elmfire has been utilized in interpretation of experimental data obtained from microwave backscattering measurements, with direct measurements of micro- to macro-scale transport phenomena in the FT-2 tokamak being quantitatively reproduced by Elmfire predictions [3, 4]. As a support for this work, we present some investigations undertaken to improve confidence in simulation results. Simulations starting from real experimental TEXTOR profiles have been shown to include all the physics ingredients to maintain the steep density profile in H-mode. For L-mode profiles, strong GAM oscillations are observed together with strongly correlated oscillatory particle flux which leads to profile relaxation [5]. Here we utilize these simulations for sensitivity analysis of E_r and χ_i.

Generally gyrokinetic investigations of neo-classical processes have been obtained potential flux surface averaging, eliminating all modes except the $(0, 0)$ zonal mode in simulations. This way turbulent modes which occupy the $k_\perp \rho \simeq 0.1-0.3$ region are eliminated, and only neo-classical processes are retained. The pure flux surface averaged potential eliminates geodesic curvature and finite Larmor radius effects that are important for the dynamics of the GAM oscillations [6, 8]. Therefore the end state of such simulations is not an true equilibrium with respect to GAM oscillations, and it is debatable if even an equilibrium of the radial electric field dynamics is obtained. The GAM oscillations exhibit the Rosenbluth residual and more complicated dynamics arises due to impurity-ion parallel friction [7]. Hence, a novel technique for solving quasi-neutrality for a neo-classically restricted plasma is proposed.

In addition to energy and momentum conservation properties of interpolation and time integration techniques, one important cause of numerical accuracy in PIC simulations is due to sampling error. In total f simulation, random noise is high from the start-up, but evolves differently in time compared to delta f simulations. Equal particle weights are used in the simulation, and growth of noise in time is more related to loss of resonant particles in the phase space, which is replenished by binary collisions. This divergence of particle weight variation makes relative disadvantage of the total f algorithm, with constant weights, to diminish in a long time scale simulations. In the present work, the effect of sampling error on E_r and χ_i are shown. For sufficient particle numbers, we observe a convergence of these quantities.

Gyrokinetic particle simulations may be restricted to neo-classical processes by averaging in tokamak plasmas. While this is usually performed by taking only the flux-surface average, it has been observed that the simple flux-surface averaging results in a non-equilibrium distribution function that kick-starts a geodesic acoustic oscillation (GAM) when the simulation is continued without averaging. In addition to the GAM oscillation dynamics, poloidal asymmetry of the electric field is important impurity dynamics, which is not properly captured by a pure flux-surface average. Non-equilibriation of the distribution function may be corrected by including the side-bands of the $n = 0$ mode. In this work we propose an orthogonal Fourier basis filtering technique which takes the non-zonal component into account in the electric field, thus removing the spurious GAM oscillation which arises when the simulation is continued without averaging.

2 Inclusion of polarization to particle density

The gyrokinetic equations of motion, Poisson equation, and exact energy and momentum conservation laws were derived in [2] based on the reduced-phase-space Lagrangian and inverse Kruskal iteration. This method allows for the inclusion of the polarization density into the particle density directly. Quasineutrality can therefore directly be evaluated by $Z\tilde{n}_i - n_e$; the gyroaveraged ion density and electron density.

In ELMFIRE , the gyrocenter motion of ions and the guiding center motion of electrons are followed by an implicit-explicit integration scheme [1]. The implicit time integration, i.e., of the ion polarization drift and the electron parallel acceleration by $\vec{E}\cdot\hat{b}$, is utilized for solving the electric potential from the quasi-neutrality condition. A second-order implicit time integration scheme has been recently introduced for the electron parallel acceleration by $\vec{E}\cdot\hat{b}$, to alleviate numerical electron heating in ELMFIRE simulations.

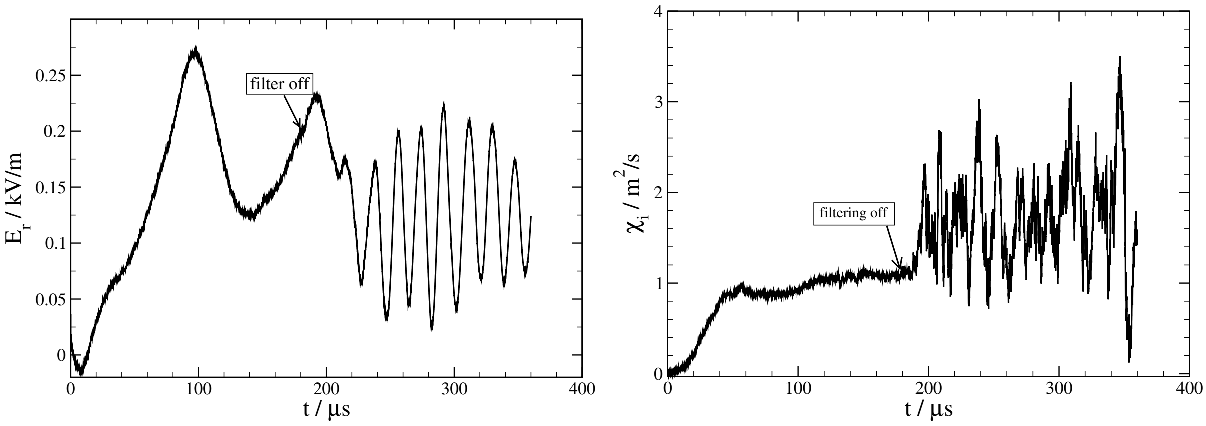

FIG. 1: Simulation of χ_i with dynamic equilibriation of the distribution function through filtering, which is turned off at $180\,\mu s$.

3 Restriction of a gyrokinetic PIC to NC processes

In the field frequently only flux surface averaged potentials are evolved (see, for example [10]) when gyro-kinetic codes are restricted to neo-classical physics. The flux surface averaged potential does not allow all geodesic curvature and finite Larmor radius effects to be included, which affect the dynamics of geodesic acoustic oscillations [6, 15]. For this reason, we have applied a technique of averaging the polarization equation starting from the charge separation between electrons and ions which eliminates the turbulent modes but retains the effects of finite Larmor radius and parallel pressure gradients on the neo-classical equilibrium.

In ELMFIRE the polarization operator is constructed so as to have polarization motion of the particles balance any charge separation, which may be shown to be equivalent to the more widely used approach of separating the polarization density from ion density. Also the parallel electric non-linearity contributes to charge neutrality. These differences complicate filtering, however, because the electric field solved from polarization (and parallel motion) needs to be consistent with charge changes locally, and as such may not be separately (outside the solution of the electric potential) averaged. Therefore neo-classical restriction implies solving the quasi-neutrality condition for the Fourier basis support.

The field-line following co-ordinate system $(r, \chi(\theta_w), \zeta)$ used in the ELMFIRE code is non-orthogonal, and as such is more cumbersome in filtering applications. The equivalent basis for the toroidal functions (omitting the radial expansion) can be expressed as the standard 2D Fourier basis $f(r, \theta_w, \phi) = \sum_{m,n} f_{m,n}(r;t)e^{i(m\theta_w + n\phi)}$, where (m, n) is the wavenumber space restricted by the support of the field line following basis. This condition is given by $-\frac{N_z}{2} < m\iota - n \leq \frac{N_z}{2}$, where N_z is the number of grid points in the parallel direction and ι is the rotational transform. While the radial potential is not developed in terms of harmonics, the eigenfunctions are orthogonal with respect to natural norm. For neo-classical investigations we generally adopt $n \equiv 0$. In figure 1 we show, for the case considered in Ref. [3], that turning off the filtering regime leaves the system dynamically stable for GAM oscillations, but allows turbulence to develop (which later drives GAM oscillations). The subtle balance in parallel dynamics in the tokamak frequently produces situations where simple flux-surface averaging is insufficient for capturing the crucial aspects of neo-classical physics [7], especially when impurities are included in simulations. The Fourier filtering technique is used for obtaining the restricted neo-classical equilibrium first, before turbulence is allowed to develop; in contrast to our earlier work [14], where both develop concurrently from initialization.

4 Conservation of energy and momentum

The conservation of the toroidal angular momentum in an axisymmetric FT-2 model magnetic configuration was investigated both in the presence of plasma turbulence as well as in the neoclassical limit [12,13]. Trivial implementation of the momentum conserving scheme is frought with major numerical troubles, but with appropriate modifications the accuracy of conservation was found to lie within the accuracy of the solver for the gyrokinetic Poisson equation, and most importantly, transport over the simulation boundaries. The time evolution of toroidal angular momentum is compared between different discretizations in figure 2 over the transport time scale and over the diagnosed plasma region. Energy conservation depends most importantly on the integration accuracy of the electron parallel acceleration and the accuracy of interpolation method for the electric field (figure 3). With current techniques of integration the relative accuracy of 10^{-3} for the electron parallel acceleration can be obtained over an energy confinement time when kinetic electrons are used. Numerical heating/cooling determines the accuracy of energy conservation and is caused by the strength of noise/random force fluctuation. Therefore, energy conservation seems to be dependent on the particle number per grid cell rather than the accuracy of diagnosing in/outflow of the energy flux over simulation boundaries [13].

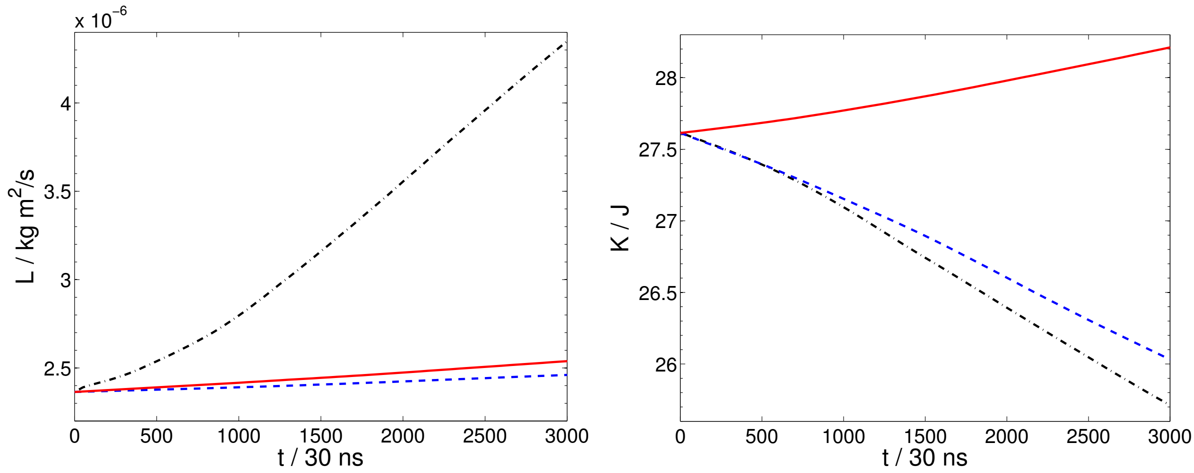

FIG. 2: Accuracy of the conservation of toroidal angular momentum (left) and energy (right) in a turbulent ELMFIRE *simulation. The black dash-dot line refers to energy conserving interpolation scheme with 1st order time stepping, the blue dashed line to momentum conserving interpolation scheme with 1st order time stepping, and the red solid to momentum conserving interpolation with 2nd order time stepping.*

5 Sampling error and transport convergence

As ELMFIRE solves the gyrokinetic equations with a Monte Carlo method, its results suffer from statistical noise coming from the fact of using a finite number of test particles. Noise production in PIC codes has been widely studied (e.g., references [9,11,15]). Simulations of ETG instability have shown the possibility of noise strongly affecting growth rates, and as such, the noise characteristics of simulations need to be investigated with particle number convergence tests. We present improved convergence of E_r an χ_i with particle number in figure 4 and figure 5 for two different parameter sets. In figure 5, which exhibits strong GAM oscillations, we observe a phase shift due to initial conditions. In all cases perfect convergence of physical quantities may not be obtained, and convergence may need to be considered on a more statistical basis. We have investigated the Cyclone Base case [16] results obtained earlier for ELMFIRE with improved noise characteristics in figure 6, which show convergence to the LLNL curve. Without particle and heat sources and sinks the linear drive is exhausted due to relaxation of profiles and transport wanes.

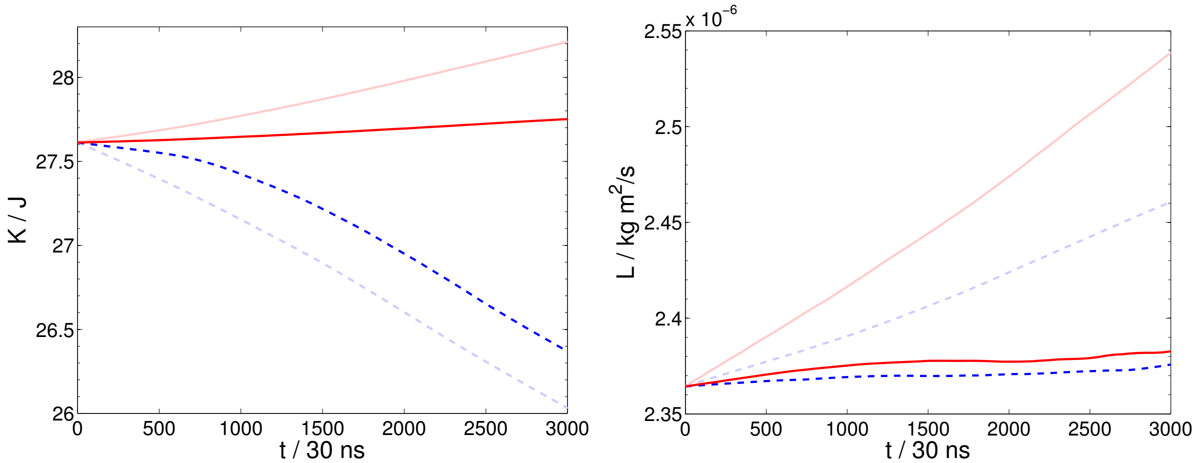

FIG. 3: Accuracy of the conservation of toroidal angular momentum (left) and energy (right) with respect to particle number. The bright lines correspond to 4400 particles per grid cell and the faint lines to 1100 particles per grid cell. The line coding corresponds to Fig. 2.

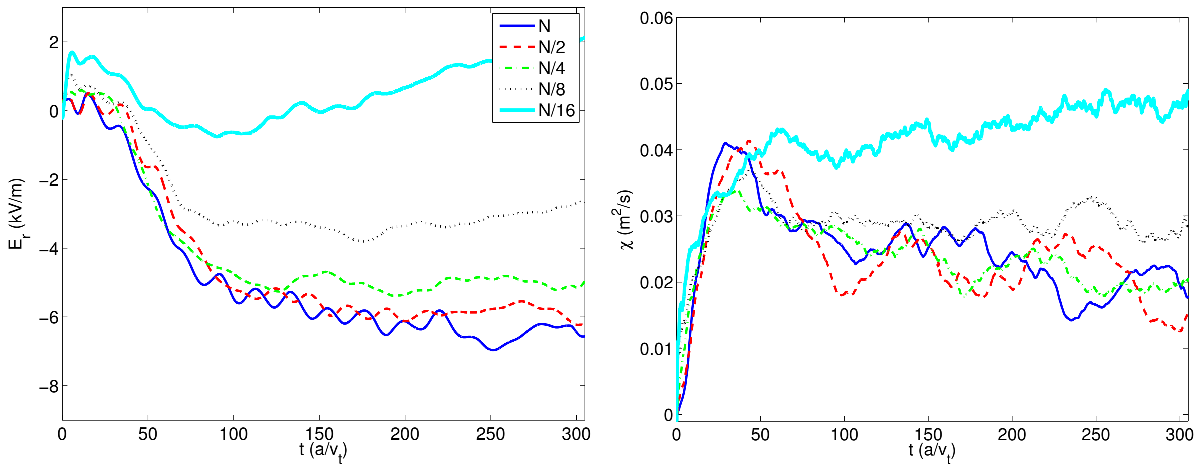

FIG. 4: Particle number convergence with respect to E_r and χ_i for the case considered in FEC'06 [14].

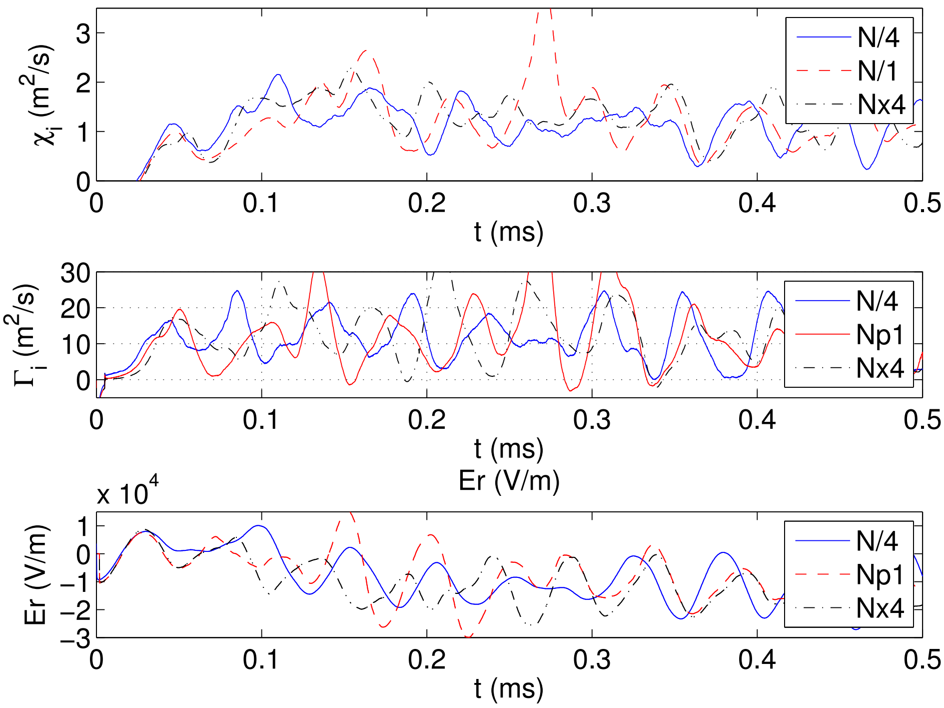

FIG. 5: Particle number convergence with respect to E_r, χ_i and Γ_i is illustrated for an L-mode case based on TEXTOR parameters [5]. The curves show similar behavior, but time evolution is sensitive on the initial value. This has been later verified also by comparing simulations where the random numbers are initialized differently; the oscillation phase changes.

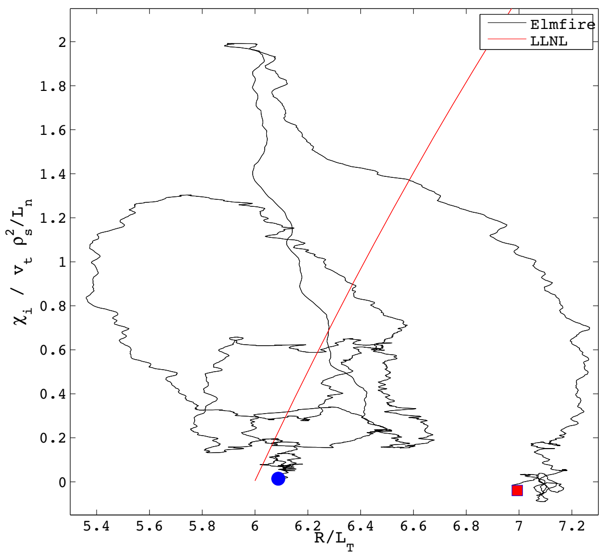

FIG. 6: Evolution of transport as a function of R/L_T starting from 6.9*, with the LLNL scaling curve. The curve begins at* □ *and ends at* ⊙.

6 Conclusions

In this work we give an overview of some of the confidence building excercises that have been performed while investigating comparisons of Elmfire results to experimental results of FT-2 and TEXTOR. These include investigations of conserved properties, such as momentum and energy, and effect of sampling error on simulation results.

We develop a filtering technique that evolves the neo-classical equilibrium without the presence of turbulence, while allowing the continuation of such simulations with full turbulence later on. The flux-surface averaging filter widely used does not produce a dynamical neo-classical equilibrium.

We present also transport convergence for the marginally unstable Cyclone Base case, with termination near the non-linear stabilization regime widely referred to as the *Dimits shift*.

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