

Advanced energetic particle transport models

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Summary. — The ATEP (advanced energetic particle transport models) EUROfusion project focuses on developing advanced transport models for energetic particles in reactor-relevant fusion plasmas. Within this project, a theoretical framework has been established to study gyrokinetic transport of energetic particles in the phase space. The main differences with usual thermal plasma transport analysis have been discussed, with special emphasis on the assumption of scale separations between fluctuations and equilibrium meso-scale corrugations as well as non-Maxwellian features. This theory relies on a redefinition (renormalization) of plasma equilibrium in the presence of a finite level of electromagnetic fluctuations known as the Zonal State. A set of equations describing its evolution consistently with the linear mode structures calculated by means of linear gyrokinetic codes like DAEPS (local) and LIGKA (global) have been integrated into the ITER Integrated Modelling and Analysis Suite (IMAS). Its accuracy is ensured through a verification against nonlinear global gyrokinetic simulations codes like ORB5. Here, the physics foundations of the theoretical framework are presented along with applications to cases of practical interest, adopting numerical simulation tools that have been developed within the ATEP project.

1. – Introduction

Traditionally, fusion plasma studies assume slowly evolving local Maxwellian equilibria, leading to 1D advection-diffusion transport equations that describe the evolution of density and temperature radial profiles observed experimentally, see, *e.g.*, ref. [1]. However, for describing the dynamics of energetic particles (EPs) and the physics of burning plasmas, equilibrium and transport descriptions must be extended to account for non Maxwellian distribution functions. In previous studies, see, *e.g.*, ref. [2], we have shown that a proper generalization of the distribution function characterizing the plasma equilibrium can be obtained by introducing the concept of Phase Space Zonal Structures [3-5] (PSZS), that is derived through a multi-scale perturbation theory. PSZS represent slowly

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evolving structures in the phase space that are not affected by fast collisionless dissipation. This approach enables a self-consistent description of equilibrium modifications on meso-scales between the characteristic times and lengths of turbulent fluctuations and the original equilibrium while taking into account deviations from the reference distribution function caused by resonant transport. In this framework, local Maxwellian equilibria are just a particular limiting case that is obtained when sources and collisions are in balance and characteristic orbit widths are small compared with the equilibrium length scales. More generally, however, equilibrium particle distribution functions can deviate from local thermodynamic equilibrium and must be computed. By calculating PSZS moments, standard transport equations can be recovered in the appropriate limits. In our previous works we have shown that an accurate representation of PSZS is crucially important to calculate a new electromagnetic kinetic equilibrium that we dubbed Zonal State [6]. A phase space transport workflow, similar to conventional advection-diffusion models, is therefore necessary to study the complex physics of burning plasmas, where EP dynamics plays a crucial role. Unlike traditional transport analyses, which rely on conventional scale separation assumptions, this requires understanding fluctuations and equilibrium meso-scale corrugations, particularly in the presence of non-Maxwellian features. In this context, fluxes must be defined in the phase space.

In the following, we will introduce the fundamental concept of PSZS and demonstrate some key results from a proof-of-principle transport workflow named ATEP. This workflow integrates stability analyses using linear gyrokinetic codes such as DAEPS (local) and LIGKA (global) and its accuracy is demonstrated through validation against global gyrokinetic simulations, showing its capability of making realistic predictions for next generation reactor-relevant Tokamaks.

2. – Governing equations

Since the PSZS concept [2-5] is proposed as a generalization of the local Maxwellian equilibrium, PSZS are “slowly evolving” by construction, that is, they must be unaffected by collisionless dissipation mechanisms like Landau damping. To achieve this, PSZS are computed using a two-step averaging procedure. First, an average is taken along the guiding center equilibrium orbits. Then, any remaining fast spatiotemporal variation is filtered out (for example, at or above the characteristic frequency of the fluctuations). Consequently, PSZS depend solely on the equilibrium invariants of motion, such as the energy $\mathcal{E}_0 = v^2/2$, magnetic moment $\mu = v_\perp^2/2B_0$, and toroidal angular momentum $P_\phi = e/c(RB_\phi v_\phi/\Omega - \psi) \sim e/c(RB_\phi v_\parallel/\Omega - \psi)$ all normalized per unit of mass. The evolution of PSZS can be expressed using these invariants as phase-space coordinates.

We introduce the phase space coordinates $\mathbf{Z} = (\theta, \zeta, P_\phi, \mathcal{E}_0, \mu)$, where θ and ζ represent the poloidal and toroidal magnetic flux coordinates, respectively. We now decompose phase-space velocity in the gyrokinetic equation as $\dot{\mathbf{Z}} = \dot{\mathbf{Z}}_0 + \delta\dot{\mathbf{Z}}$, where $\dot{\mathbf{Z}}_0$ represents the integrable motion in the reference magnetic field, and $\delta\dot{\mathbf{Z}}$ accounts for fluctuations spontaneously produced by plasma dynamics. This decomposition is applicable to nearly integrable Hamiltonian systems and requires that the reference equilibrium varies slowly in time. Accordingly, the gyrokinetic equation can be written in conservative form as:

$$(1) \quad \frac{\partial}{\partial t}(DF) + \frac{\partial}{\partial \mathbf{Z}} \cdot (D\dot{\mathbf{Z}}_0 F) + \frac{\partial}{\partial \mathbf{Z}} \cdot (D\delta\dot{\mathbf{Z}} F) = 0,$$

where D is the velocity space Jacobian⁽¹⁾ and F the gyro-center distribution function [7]. To simplify the analysis, we assume that the equilibrium radial electric field, if present, corresponds to a sufficiently slow $E \times B$ flow consistent with the gyrokinetic ordering and that can be incorporated into the perturbed radial electric field.

The zonal distribution function F_z is defined in the following as the toroidally symmetric part of the full distribution function F . This is the natural starting point for defining an equilibrium distribution in Tokamak plasmas. For the equilibrium axisymmetric magnetic field, without loss of generality, we assume $\mathbf{B}_0 = \hat{F}\nabla\phi + \nabla\phi \times \nabla\psi$, where $\hat{F} = RB_\phi$, and ϕ is the toroidal angle related to ζ by $\zeta = \phi - \nu(\psi, \theta)$, with $\nu(\psi, \theta)$ chosen such that the magnetic flux coordinates are characterized by straight magnetic field lines. We now focus on re-writing the term describing the equilibrium motion in the zonal component of eq. (1):

$$(2) \quad \frac{\partial}{\partial \mathbf{Z}} \cdot (D\dot{\mathbf{Z}}_0 F)_z = \nabla \cdot (D\dot{\mathbf{X}}_0 F)_z = \frac{1}{\mathcal{J}_{P_\phi}} \frac{\partial}{\partial \theta} (D\mathcal{J}_{P_\phi} F \dot{\mathbf{X}}_0 \cdot \nabla \theta)_z,$$

where $\mathcal{J}_{P_\phi} = \mathcal{J}(\partial P_\phi / \partial \psi)^{-1}$ and $\mathcal{J} = (\nabla \zeta \cdot \nabla \psi \times \nabla \theta)^{-1}$ is the Jacobian in flux coordinates. In deriving this expression, we have used the toroidal symmetry of the reference state along with the conservation of P_ϕ and the energy characterizing particle motion in the equilibrium magnetic field, *i.e.*, respectively $\dot{\mathbf{X}}_0 \cdot \nabla P_\phi = 0$ and $\dot{\mathcal{E}}_0 = 0$.

Next, we average the zonal component of eq. (1) while keeping P_ϕ using \mathcal{J}_{P_ϕ} as weight. This averaging naturally eliminates the second term in eq. (1). Assuming that the reference magnetic equilibrium is slowly evolving; *e.g.*, on the resistive current diffusion time, we obtain:

$$(3) \quad \partial_t \oint d\theta \mathcal{J}_{P_\phi} D F_z + \oint d\theta \mathcal{J}_{P_\phi} \frac{\partial}{\partial \mathbf{Z}} \cdot (D\delta\dot{\mathbf{Z}}F)_z = 0.$$

Recall, see, *e.g.*, ref. [7], that the equilibrium motion is governed by: $\dot{\psi} = -v_{\parallel} \partial_\theta \bar{\psi} / (\mathcal{J} B_{\parallel}^*)$, where $\bar{\psi} = -(c/e)P_\phi$, $\dot{\theta} = v_{\parallel} \partial_\psi \bar{\psi} / (\mathcal{J} B_{\parallel}^*)$ and $D = B_{\parallel}^* / |v_{\parallel}|$, with $B_{\parallel}^* \equiv \mathbf{B}^* \cdot \mathbf{b}$, $\mathbf{b} \equiv \mathbf{B}_0 / B_0$, $\mathbf{B}^* \equiv \nabla \times \mathbf{A}^*$, $(e/c)\mathbf{A}^* \equiv (e/c)\mathbf{A}_0 + m(v_{\parallel} \mathbf{b})$, $\mathbf{B}_0 \equiv \nabla \times \mathbf{A}_0$. By direct substitution of these expressions, it can be shown that the averaging applied in eq. (3) correspond to the following equilibrium orbit average:

$$(4) \quad \overline{(\dots)}^{(0)} = \tau_b^{-1} \oint d\theta (\dots) / \dot{\theta},$$

where the time required by the particle to close a poloidal loop (bounce time) is given by $\tau_b = \oint d\theta / \dot{\theta}$. As explained with major details in ref. [6], in the limit of vanishing orbit width size, this correspond to the usual bounce averaging operation.

As explained in ref. [2], deriving the PSZS governing equation requires extracting the macro-/meso-scopic components of eq. (3):

$$(5) \quad \frac{\partial}{\partial t} \overline{F_0}^{(0)} + \frac{1}{\tau_b} \left[\frac{\partial}{\partial P_\phi} \overline{(\tau_b \delta \dot{P}_\phi \delta F)}_z^{(0)} + \frac{\partial}{\partial \mathcal{E}} \overline{(\tau_b \delta \dot{\mathcal{E}} \delta F)}_z^{(0)} \right]_S = \overline{C_S^g}^{(0)} + \overline{S_S}^{(0)}.$$

⁽¹⁾ The explicit expression for D will be given below.

Here, $[\dots]_S$ describes an appropriate spatio-temporal averaging procedure, the choice of which depends on the features of the fluctuation spectrum under investigation. The right-hand side includes source and collision terms.

Having introduced the concept of PSZS, we now decompose the gyrocenter particle response and, consequently, the zonal component of the gyrokinetic distribution function F_z , into contribution due to different underlying physical processes. Specifically, we write:

$$(6) \quad F_z = \overline{F_z}^{(O)} + \delta\tilde{F}_z = \overline{F_0}^{(O)} + \delta\overline{F_z}^{(O)} + \delta\tilde{F}_z.$$

Following ref. [6], the individual terms of this decomposition can be interpreted as follows: $\overline{F_0}^{(O)}$ represents the slowly evolving equilibrium, $\delta\overline{F_z}^{(O)}$ captures microscale corrugations of the equilibrium often referred to as ‘‘neighboring equilibria’’ [8], while $\delta\tilde{F}_z$ is the residual term, which by construction has zero orbit average.

3. – ATEP code

In ref. [9], eq. (5) was implemented in a numerical workflow in order to simulate the evolution of the distribution function based in realistic Tokamak experimental conditions. At first, a constant-amplitude fluctuation with an assigned fluctuation spectrum is considered at each time step.

The evolution of the PSZS can be described in terms of a flow velocity $\overline{\mathbf{v}}^{(O)} \equiv (v_{P_\phi}, v_{\mathcal{E}})$. The details of the numerical procedure required to calculate $\overline{\mathbf{v}}^{(O)}$ are outside the scope of this review and are discussed in ref. [9] but they can be schematically described as follow. First, the region of interest in the phase space $(\theta, \zeta, P_\phi, \mathcal{E}_0, \mu)$ is covered with markers. Then, their motion is tracked over a short time interval Δt . The displacements in the P_ϕ and \mathcal{E} coordinates are recorded. By averaging over tracers starting with the same initial value of P_ϕ , \mathcal{E} and μ and dividing by Δt , the components of $\overline{\mathbf{v}}^{(O)}$ can be determined. On the same grid, the tracers equilibrium motion, *i.e.*, in the absence of fluctuations, is fully characterized, allowing to discriminate between trapped particles which are reflected by the magnetic mirror effect in regions of higher magnetic field strength and passing particles. The motion of the tracers is calculated in the presence of the fluctuating electromagnetic fields solved by the LIGKA code [10], a global linear GK code capable of describing Alfvén eigenmodes in realistic experimental geometries.

In fig. 1, we present a simple example: the results obtained for a Toroidal Alfvén eigenmode (TAE) with toroidal mode number $n = 13$ using an ITER equilibrium [11]. Since LIGKA solves the linearized gyrokinetic equations, it does not determine the mode amplitude; therefore, we have assumed $\delta B/B = 5 \times 10^{-6}$ as done in ref. [9]. In particular, in fig. 1, we show v_{P_ϕ} for different particle populations. As expected, the response of trapped and passing particles is completely different and sharply localized in the phase space due to the resonant wave particle interactions. These phase-space localized contributions imply that properly describing the plasma equilibrium evolution requires solving the PSZS governing equation.

To consistently evolve the PSZS, an equation for the fluctuation amplitude evolution must be provided. Following ref. [9], as a simple example, we introduce an energy balance between the wave amplitude spectrum and phase space flows:

$$(7) \quad \frac{d}{dt} (E_p + \sum_k W_k) = -2 \sum_k \gamma_{d,k} W_k,$$

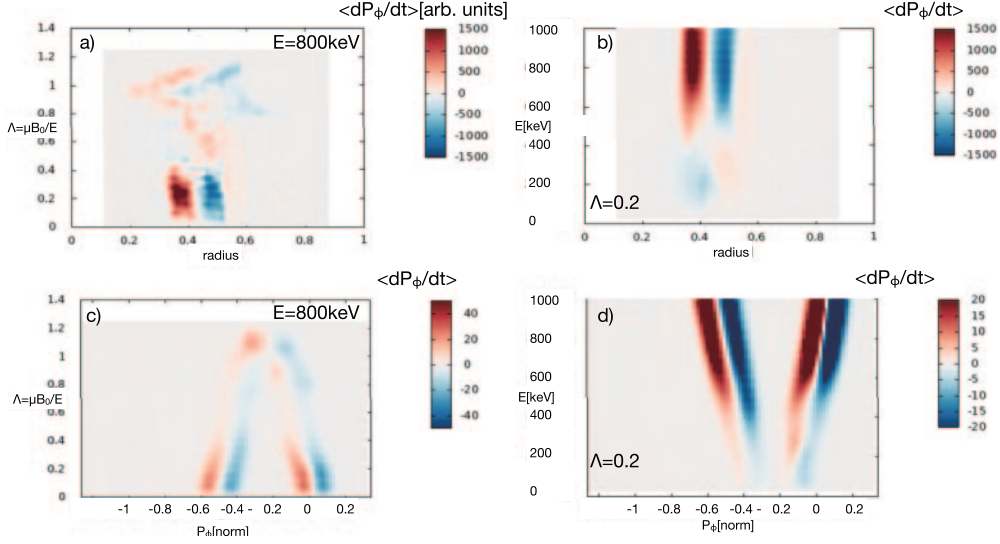


Fig. 1. $-v_{P_\phi} \equiv \langle dP_\phi/dt \rangle$ expressed in arbitrary units is presented for a single $n = 13$ Toroidal Alfvén eigenmode with $\delta B/B = 5 \cdot 10^{-6}$. This is shown as a function of the real space radial coordinate (panels (a) and (b)) and as a function of the coordinate P_ϕ (panels (c) and (d)). Different phase-space slices are considered: left panels (a),(c): in the radius- Λ plane for the Energy $E \equiv m_i \mathcal{E}_0 = 800$ keV with m_i being the mass of the considered ion species; right panels (b),(d): in the radius-ES plane for $\Lambda = \mu B_0/\mathcal{E}_0 = 0.2$. The radial coordinate is given in terms of the square root of the normalized poloidal flux.

where $\sum_k W_k$ is the total wave energy as a superposition of k linear eigenmodes, $\gamma_{d,k}$ are their corresponding damping rates as calculated by the linear code LIGKA, and E_p denotes the kinetic energy of the particle distribution. In this model, the flow velocity is pre-calculated for different perturbation amplitudes and interpolated during the time evolution of the system.

In fig. 2, we present the results from a simple run of ATEP considering only one eigenmode. During the evolution, the shape of the wave spectrum remains fixed while the amplitude evolves according to eq. (7) (see the right panel). For this plot, only the contribution from the most resonant particles are included. In particular the left panel illustrates transport in a section of the Tokamak where the initial markers are colored according to the relative modification of the PSZS caused by advection. The critical role of accurately describing the PSZS in kinetic simulations is stressed by the fact that, as expected, zonal density perturbations are coupled to its evolution. The related zonal electromagnetic fields, in turn, have been shown to crucially impact the turbulence saturation level in fusion plasmas simulations and experiments.

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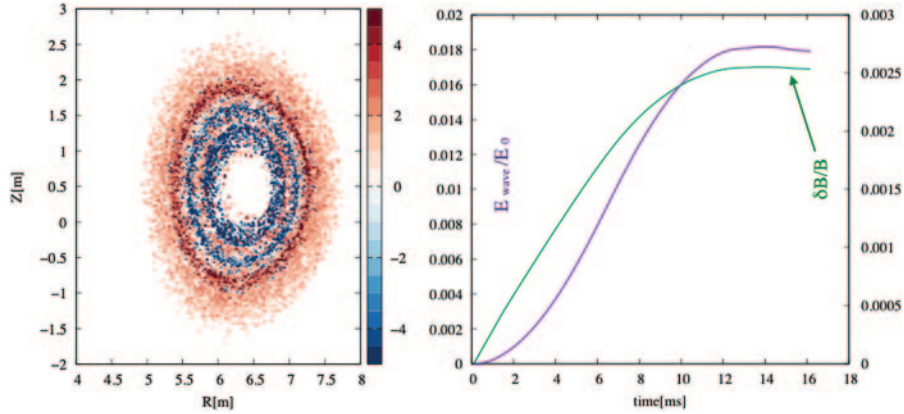


Fig. 2. – Left: mapping back the PSZS to marker space shows that the transport equation indeed introduces a zonal (toroidally symmetric) density perturbation to F_{EP} , here represented as the change of marker weights (%) (color bar). For this plot only the most resonant particles with $E > 500 \text{ keV}$ and $\Lambda < 0.3$ were chosen. Right: the normalised wave energy $E_{wave}(t)/E_0$ and $\delta B(t)/B_0$ are allowed to evolve dynamically according to the energy balance eq. (7). This figure is taken from ref. [9].

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