

## Theory and simulation of Phase Space transport in burning plasmas

M. V. Falessi<sup>1,2</sup>, Ph. Lauber<sup>3</sup>, F. Zonca<sup>1</sup>, A. Bottino<sup>3</sup>, L. Chen<sup>4</sup>, Th. Hayward-Schneider<sup>3</sup>, G. Meng<sup>3</sup>, A. Mishchenko<sup>5</sup>, Z. Qiu<sup>6</sup>, G. Wei<sup>4</sup>

<sup>1</sup>ENEA, Nuclear Department, Rome, Italy

<sup>2</sup>Instituto Nazionale di Fisica Nucleare, Sezione di Roma, Rome, Italy

<sup>3</sup>Max Planck, Institute for Plasma Physics, Garching, Germany

<sup>4</sup>Zhejiang Univ., Inst. for Fusion Theory and Simulation and School of Physics, Hangzhou, China

<sup>5</sup>Max Planck, Institute for Plasma Physics, Greifswald, Germany

<sup>6</sup>Chinese Academy of Sciences, Institute of Plasma Physics, Hefei, China

### Introduction

Traditionally transport studies of fusion plasmas rely on local Maxwellian equilibria and 1D equations governing their temporal evolution, but this approach is insufficient for capturing the complex dynamics of energetic particles and, more generally, burning plasmas [1-4,6,7]. To address this, the concept of Phase Space Zonal Structures (PSZS) has been introduced, representing slowly evolving, non-Maxwellian features of the distribution function derived via multi-scale perturbation theory [5]. PSZS allows for a self-consistent description of equilibrium modifications at meso-scales, crucial for understanding resonant transport effects. These structures enable the recovery of the usual transport equations [6] and allow us to define the concept of Zonal State (ZS), that is the plasma nonlinear equilibrium calculated self-consistently with the PSZS. This paper reviews the concepts of PSZS and ZS and describes the ATEP workflow [8], validated against global simulations, for modeling phase space transport in future fusion reactors.

### Governing equations

Since the PSZS concept 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  $\theta$  and  $\zeta$  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:

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

where  $D$  is the velocity space Jacobian and  $F$  the gyro-center distribution function. 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  $\phi$  is the toroidal angle related to  $\zeta$  by  $\zeta = \phi - v(\psi, \theta)$ , with  $v(\psi, \theta)$  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 the previous equation:

$$\frac{\partial}{\partial \mathbf{Z}} \cdot (D \mathbf{Z}_0 F)_z = \nabla \cdot (D \mathbf{X}_0 F)_z = \frac{1}{J_{P_\phi}} \frac{\partial}{\partial \theta} (D J_{P_\phi} F \mathbf{X}_0 \cdot \nabla \theta)_z$$

Where  $J_{P_\phi} = J \left( \frac{\partial P_\phi}{\partial \psi} \right)^{-1}$  and  $J = (\nabla \zeta \cdot (\nabla \psi \times \nabla \theta))^{-1}$  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  $P_\phi$  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 the Gyrokinetic equation while keeping  $P_\phi$  using  $J_{P_\phi}$  as weight. Assuming that the reference magnetic equilibrium is slowly evolving, e.g., on the resistive current diffusion time, we obtain:

$$\partial_t \oint d\theta J_{P_\phi} D F_z + \oint d\theta J_{P_\phi} \frac{\partial}{\partial \mathbf{Z}} \cdot (D \delta \mathbf{Z} F)_z = 0$$

Recall, that the equilibrium motion is governed by:  $\psi = -\frac{v_\parallel \partial_\theta \bar{\psi}}{J B_\parallel^*}$  where  $\bar{\psi} = -(c/e)P_\phi$ ,  $\theta = \frac{v_\parallel \partial_\psi \bar{\psi}}{J B_\parallel^*}$  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 correspond to the following equilibrium orbit average:  $\tau_b^{-1} \oint d\theta / \dot{\theta}$  where the time required by the particle to close a poloidal loop (bounce time) is given by:  $\tau_b = \oint d\theta / \dot{\theta}$ . In the limit of vanishing orbit width size, this corresponds to the usual bounce averaging operation.

As explained in Ref. [4], deriving the PSZS governing equation requires extracting the macro-/mesoscopic components of the previous expression:

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

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.

## ATEP code

In Ref. [8] the PSZS equation was implemented in a numerical workflow to simulate the evolution of the distribution function in realistic Tokamak experimental conditions including also collisional

transport [1]. 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 with components  $(v_{P_\phi}, v_\varepsilon)$ . The details of the numerical procedure required to calculate this velocity are outside the scope of this review and are discussed in Ref. [8] but they can be schematically described as follow. First, the region of interest in the phase space  $(\theta, \zeta, P_\phi, \varepsilon_0, \mu)$  is covered with markers. Then, their motion is tracked over a short time interval  $\Delta t$ . The displacements in the  $P_\phi$  and  $\varepsilon$  coordinates are recorded. By averaging over tracers starting with the same initial value of  $P_\phi$ ,  $\varepsilon$  and  $\mu$  and dividing by  $\Delta t$ ,  $(v_{P_\phi}, v_\varepsilon)$  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 [9], 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. 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. [8]. In Fig. 1, we show  $v_{P_\phi}$  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.

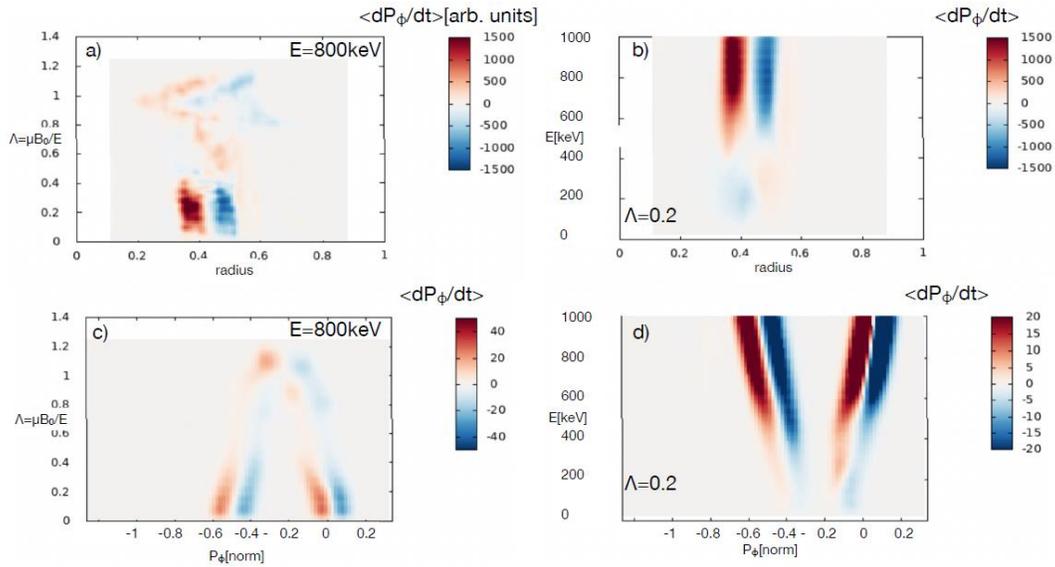


Fig 1.  $v_{P_\phi} \equiv \langle dP_\phi/dt \rangle$  expressed in arbitrary units is presented for a single  $n = 13$  Toroidal Alfvén eigenmode with  $\delta B/B = 5 \cdot 10^{-6}$ . This is shown as a function of the real space radial coordinate (panels a) and b)) and as a function of the coordinate  $P_\phi$  (panels c) and d)). Different phase-space slices are considered: left panels a), c): in the radius- $\Lambda$  plane for the Energy  $E \equiv m_i \varepsilon_0 = 800 \text{ keV}$  with  $m_i$  being the mass of the considered ion species; right panels b), d): in the radius -  $\varepsilon_0$  plane for  $\Lambda = \mu B_0/\varepsilon_0 = 0.2$ . The radial coordinate is given in terms of the square root of the normalized poloidal flux.

To consistently evolve the PSZS, an equation for the fluctuation amplitude evolution must be provided. Following Ref. [8], as a simple example, we introduce an energy balance between the wave amplitude spectrum and phase space flows:

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

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 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 the previous expression (see the right panel). For this plot, only the contribution from the most resonant particles is included. 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 their evolution. The related zonal electromagnetic fields, in turn, have been shown to crucially impact the turbulence saturation level in fusion plasmas simulations and experiments.

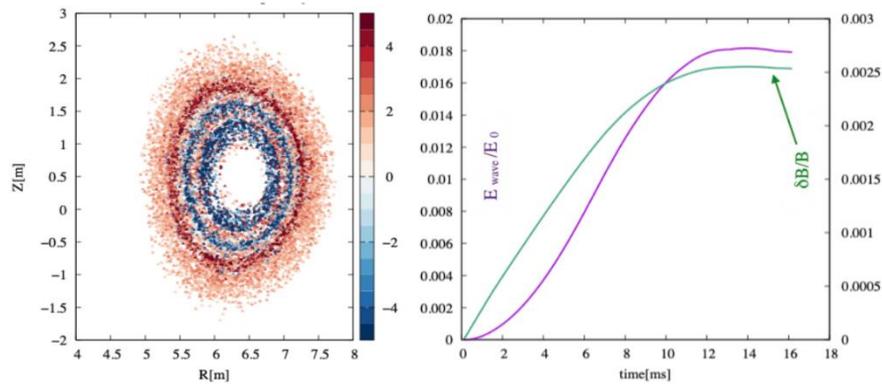


Fig 2. Left: mapping back the PSZS to marker space shows that the transport equation indeed introduces a zonal (toroidally symmetric) density perturbation to  $F_{EP}$ , here represented as the change of marker weights [%] (color bar). For this plot only the most resonant particles with  $E > 500\text{keV}$  and  $\Lambda < 0.3$  were chosen. Right: the normalised wave energy  $E_{\text{wave}}(t)/E_0$  and  $\delta B(t)/B_0$  are allowed to evolve dynamically according to the energy balance. This figure is taken from Ref.[8] .

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