Transport in fusion plasmas: is the tail wagging the dog?

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Turbulent plasmas notably self-organize to higher energy states upon application of additional free energy sources or modification of edge operating conditions. Mechanisms whereby such bifurcations occur have been actively debated for decades. Enhanced confinement occurs at the plasma edge, where a shortfall of predicted turbulence intensity has been puzzling scientists for decades. We show, from the primitive kinetic equations that both problems are connected and that interplay of confined plasma turbulence with its material boundaries is essential to curing the shortfall of predicted turbulence and to triggering spontaneous transport barrier onset at the plasma edge. Both problems determine access to improved confinement and are central to fusion research. A comprehensive discussion of the underlying mechanisms is proposed. These results, highly relevant to the quest for magnetic fusion may also be generic to many problems in fluids and plasmas where turbulence self-advection is active.

In the quest for magnetic confinement fusion, field geometry plays an important role. Magnetic field lines in tokamaks or stellarators are built such as to trace out closed toroidal flux surfaces with a high degree of symmetry. Field symmetry is known to bolster confinement, enabling entrapment of the ionised plasma. Symmetry breaking however is common and usually results in net particle, energy or momentum sinks and ultimately in degradation of confinement. In particular, toroidal symmetry in the plasma core where fusion reactions occur breaks down in the peripheral plasma as flux surfaces open up and field lines intercept material boundaries. Transition from closed to open
field lines is usually abrupt, occurs about the so-called magnetic separatrix and plays an important role for confinement.

Established practice oft distinguishes between a hot confined ‘core’ region, dense and hot, an unconfined peripheral boundary layer (the ‘Scrape-Off Layer’ or ‘SOL’) and an in-between ‘edge’ region, loosely defined, set between core and separatrix. The SOL is cold and rarefied; it starts at the magnetic separatrix and is mapped out by the open field lines which connect magnetically to the material boundaries. Core and SOL have been extensively studied, mostly independently; the edge usually serving in modelling as fixed boundary condition for both, its dynamics difficult to apprehend. Strict decoupling however between all three regions is increasingly being questioned. Tokamak plasmas are indeed prone to self-organisation and mounting evidence suggests interplay between core, edge and SOL. Realistic modelling of fusion-grade plasmas must address this delicate balance and tackle dynamics in the vicinity of the closed to open field line interface.

The near-separatrix edge region is a cornerstone of fusion research, where spontaneous transitions from low-confinement “L-mode” to high-confinement “H-mode” occur [1]. The H-mode branch of operation is one of several improved confinement states that have been experimentally discovered, re-vitalizing the fusion program towards ITER. Microturbulence dominates the transport processes in the L–mode edge. Description from first principles of the transport processes there, prior to bifurcations, is largely missing yet key to establishing whereby transport bifurcations occur.

We discuss a generic situation, based on experimental parameters where the following conundrum is found: experimentally, the edge is measured to be turbulent, with fluctuations increasing with proximity to the separatrix [2]. In contrast, local analysis of the profiles predicts convective stability in the edge and increased stability with proximity to the separatrix. The edge region would thus appear as unfit to produce or sustain a turbulent state. This opposes the experimental trend and precludes the possibility for turbulence-induced bifurcations to improved confinement. This problem was first formulated decades ago and is still often referred to as the "transport shortfall" conundrum.

We show, from the primitive kinetic equations, a possible resolution for this problem. Understanding the origin of turbulence activity in the edge requires considering the interplay between closed and open field lines. Magnetic connection to the material boundaries deeply modifies global convective stability at the separatrix. An additional source of free energy arises there, resulting in the confined
plasma being driven unstable. Fluctuations, initially localised in a narrow peripheral area of the plasma at the plasma–material boundary interface expand beyond their region of convective drive and ”spread” throughout the stable edge. Surprisingly, this narrow peripheral region controls the dynamics of much larger plasma core and edge through fluxes of turbulence activity, a case of the tail wagging the dog.

**Model equations.** – Low-frequency microturbulence in weakly collisional magnetised plasmas is appropriately described within the gyrokinetic framework [3]. The GYSELA code [4] solves the governing coupled gyrokinetic:

$$B_{\parallel}^s \frac{\partial \tilde{F}_s}{\partial t} + \nabla \cdot \left( B_{\parallel}^s \frac{d\mathbf{x}_G}{dt} \tilde{F}_s \right) + \frac{\partial}{\partial v_G \parallel} \left( B_{\parallel}^s \frac{dv_G \parallel}{dt} \tilde{F}_s \right) = B_{\parallel}^s \text{(rhs)} \quad (A-1)$$

$$\text{rhs} = C + S + D - \nu \mathcal{M}^\text{mat}(r, \theta) [\tilde{F}_s - \tilde{G}_\text{cold}] - \gamma K \left[ \tilde{F}_s - \tilde{F}_\text{F-D} \left( 1 + \frac{\langle \tilde{F}_s - \tilde{F}_\text{F-D} \rangle}{\langle \tilde{F}_\text{F-D} \rangle} \right) \right] \quad (A-2)$$

and quasi-neutrality:

$$\Delta n_e = \rho + \frac{1}{n_{e0}} \sum_s Z_s \nabla \perp \cdot \left( \frac{n_{e0}}{B_0} \nabla \perp \phi \right) \quad \text{(A-3)}$$

$$\frac{T_e}{e} \Delta n_e = \phi - \lambda \left[ 1 - \mathcal{M}^\text{SOL}(r) \right] \langle \phi \rangle_{\text{FS}} - \left[ \mathcal{M}^\text{mat}(r, \theta) - \mathcal{M}^\text{wall}(r) \right] \phi_{\text{bias}}$$

$$- \lambda \Lambda \left[ \mathcal{M}^\text{SOL}(r) - \mathcal{M}^\text{mat}(r, \theta) \right] (T_e - T_e^{b.c.}) \quad (A-4)$$

equations for the guiding-center distribution function $\tilde{F}_s$ of ion species $s$, evolved with no separation between equilibrium and perturbation in five dimensional guiding-centre space ($\mathbf{x}_G, v_G \parallel, \mu$) and time. In Eq.(A-2), $\langle \cdot \rangle = \int J_v J_x \cdot dv \mu d\theta d\varphi$, with $J_v$ and $J_x$ being the velocity and space Jacobians. The charge density of guiding-centers $\rho$ is computed as:

$$\rho(\mathbf{x}, t) = \frac{1}{n_{e0}} \sum_s Z_s \int d\mu \mathcal{J}_\mu \left[ \int J_v \, dv_G \parallel (\tilde{F}_s(\mathbf{x}, v, t) - \tilde{F}_{s,eq}(r, \theta, v_G \parallel)) \right] \quad (A-5)$$

with $\mathcal{J}_\mu$, the gyro-average operator. Notations are those of Ref.[4]. The computational domain extends from inner core ($r/a = 0$) to the material boundaries ($r/a = 1.3$). Flux- or gradient-driven dynamics may be considered. For flux-driven evolution, $\gamma K = 0$ and the distribution function evolves according to volumetric sources $S$ [5] and penalised [6, 7] heat and momentum sinks $\mathcal{M}^\text{mat}(r, \theta)$, $\mathcal{M}^\text{SOL}(r)$ and $\mathcal{M}^\text{wall}(r)$ that can mimic from poloidally-uniform boundary conditions (Case-2) to the more complex limiter and wall geometries (Case-1). The latter case allows description of the closed to open field
lines transition in the Scrape-Off Layer (SOL). Gradient-driven-like dynamics may also be considered whilst imposing $S = \mathcal{M}^{\text{mat}}(r, \theta) = \mathcal{M}^{\text{wall}}(r) = 0$. In Case-3, the target distribution function $F_{\text{D}}$ is chosen as the statistical distribution at equilibrium from flux-driven Case-2 and the relaxation rate $\gamma^K = 5.43 \times 10^{-5} \sim \gamma_{\text{lin}}/10$ is an order of magnitude smaller than the local linear turbulence growth rate $\gamma_{\text{lin}}$ at $r/a = 0.7$. Imposing $\mathcal{M}^{\text{SOL}}(r)$ as in Case-2 or cancelling this mask does not alter the dynamics which is dominated by the BGK operator [last term of Eq. (A-2)], specifically described in Ref. [8] and built such as to prevent overdamping zonal modes [9].

Penalisation [6] modifies the equations through introduction of a series of masks $\mathcal{M}^{\text{mat}}(r, \theta)$, $\mathcal{M}^{\text{SOL}}(r)$ and $\mathcal{M}^{\text{wall}}(r)$, combinations of hyperbolic tangents, adjustable in location, shape (for $\mathcal{M}^{\text{mat}}(r, \theta)$) and stiffness. They are illustrated in Fig. A-1. Electrons have a Boltzmann response modified by penalisation such that the electric potential $\phi$ in the quasi-neutrality equation is relaxed towards its expected presheath condition $\Lambda = \sqrt{m_i/m_e}$ in the SOL. Additionally, $\phi$ may be biased to $\phi^{\text{bias}}$ in the limiter ($\phi^{\text{bias}} = 0$ in the current study) and is freely evolving elsewhere. $T_e^{\text{h.c.}}$ is the cold electron temperature within limiter and wall, chosen as the minimum $T_e$ value within the computational domain, $\Lambda = \log(\sqrt{m_i/m_e})$ and coefficient $\lambda$ (set to unity in the present study) may be used to alter the inertia of the zonal potential. In the gyrokinetic equation, infinite penalisation [7] relaxes

| Tokamak volume                 | Mask                                                                 |
|--------------------------------|----------------------------------------------------------------------|
| All plasma                    | $1 - \mathcal{M}^{\text{mat}}(r, \theta)$                          |
| Closed field lines            | $1 - \mathcal{M}^{\text{SOL}}(r)$                                   |
| Scrape-Off Layer              | $\mathcal{M}^{\text{SOL}}(r) - \mathcal{M}^{\text{mat}}(r, \theta)$ |
| Material boundaries           | $\mathcal{M}^{\text{mat}}(r, \theta)$                               |
| Limiter only                  | $\mathcal{M}^{\text{mat}}(r, \theta) - \mathcal{M}^{\text{wall}}(r)$|
| Wall only                     | $\frac{\mathcal{M}^{\text{mat}}(r, \theta)}{\mathcal{M}^{\text{wall}}(r)}$ |

Fig. A-1. The various masks used for penalisation in the gyrokinetic–Poisson system.
to a target cold Maxwellian distribution function \( G_{\text{cold}} = n_w (2\pi T_w)^{-3/2} \exp[-(v_{G||}^2 + \mu B)/2T_w] \),

calibrated by low wall thermal energy \( T_w \) and target density \( n_w \). The former is constrained by
velocity-space resolution; we typically choose it an order of magnitude lower that temperature at mid
radius whilst the target density \( n_w \) is chosen so as to ensure particle conservation. This setting is
easily extrapolable to a kinetic response for electrons inside the separatrix (for \( r/a \leq 1 \)), retaining an
adiabatic electron response in the SOL. Relaxation of this assumption in the SOL is currently under
investigation [10].

**Modelling strategies: flux- and gradient-driven approaches** –

which has three major implications: (i) as touched upon above, a flux-driven framework is required
implying that profiles, flows, stresses and flux patterns are unknowns of the dynamical problem and
the main outcomes of the numerical experiment. The plasma self-organises on a fraction of a con-
finement time and alters its internal profiles in a self-consistent fashion whilst retaining memory of
this reorganisation. It opens the possibility to dynamically describe a bifurcation. In addition, (ii)
the full volume of the plasma from dense core to rarefied SOL next to the material boundaries is
resolved. Each region of the plasma volume is a priori dynamically connected to the rest so that
all parts may interplay. At last, (iii) no temporal and spatial scale separation is assumed as many
relevant scales commonly associated to ‘mean’ quantities or to ‘fluctuations’ do interplay, from the
short ion-scale Larmor radius \( \rho_i \sim 10^{-3} \text{m} \) of turbulent eddies driven by Ion Temperature Gradient
(ITG) and Trapped Electron Mode (TEM) turbulence to the global machine scale \( (L \sim 1 \text{m}) \) and
intermediate gradient mesoscales \( (\sim \sqrt{\rho_i L}) \) where turbulence self-organises. Here, \( \rho_i \) denotes the ion
Larmor radius. Similarly, fast turbulent motion \( (\sim 10^{-5} \text{s}) \), slower turbulent spreading \( (\sim 10^{-3} \text{s}) \) and
collisional transport \( (\sim 10^{-5} \text{s}) \), slow energy confinement equilibration \( (\sim 0.1 \text{s}) \) are treated on an equal
footing.

Such properties make the problem computationally intensive yet are instrumental to the results
discussed here. The multiple length and time scales are indeed known to interplay in the core, e.g.
through predator—prey-like dynamics between zonal flows and turbulence [11] or through the onset
of staircases [8]. As characteristic scales in the edge all become comparable due to the large gradients
of mean plasma quantities when approaching the separatrix, separations either in time or in space,
though computationally favourable in gradient-driven models become questionable. Furthermore,
the modelling perspective on turbulence changes between the plasma core and its periphery. In the confined core, provided known constraints such as the minor radius of the torus, its aspect ratio or its magnetic configuration, the central focus is on predicting the energy, momentum or particle confinement time. Diffusion in that matter is the oft-invoked paradigm for the analysis of transport. The question of estimating a confinement time is thus often recast as a problem of estimating heat, momentum or particle diffusivities. Through the argument that transport is stiff, mean gradients are thus often taken out of the dynamic feedback loops that determine transport and are assumed to be known and to act as reservoirs of free energy. Gradient-driven approaches thus allow to compute a transport matrix at a reduced numerical cost. They are the current workhorse for estimating transport in the confined core of turbulent fusion plasmas, documented objections to their implicit assumptions of locality and diffusive transport notwithstanding [12, 13]. However, when crossing the separatrix the situation is drastically modified. The confinement time is no longer the primary issue in the vicinity of the separatrix and in the scrape-off layer for it is tightly constrained by the magnetic connections to the boundaries. Cross-field transport impacts flux deposition patterns, which is of primary concern for fusion. As sources and sinks are intrinsically not uniformly distributed along the field lines, the determination of the poloidal distribution of gradients is a central question, as well as the radial propagation of turbulence on both sides of the separatrix. The edge—SOL interface thus needs addressing in a flux-driven framework.

Primitive modelling is especially useful if it strives to remain predictive, not relying upon stiffness arguments, adjustable gradients to match experimental observations. In that respect, flux-driven strives to do just this: to remain predictif.

Physical parameters and robustness. – The reference Tore Supra shot 45511 had 2MW of Ion Cyclotron Resonance Heating on top of 1MW of Ohmic heating injected in a deuterium plasma of normalised size $\rho_\ast = \rho_i/a = 1/500$ at mid radius and aspect ratio $a/R_0 = 1/3.3$, $a$ and $R_0$ being respectively the minor and major radius. The plasma current is $I_p = 0.8$MA, the magnetic field on axis is $B_0 = 2.8$T and the density and temperature at mid-radius respectively read: $n = 4 \times 10^{19}$m$^{-3}$ and $T = 0.8$keV. In GYSELA, a 3MW volumetric heat source comparable in shape to that in the experiment is injected in the central 40% of a deuterium torus of same aspect ratio. Initial density, electron and ion temperature profiles are the same as in the experiment up to the separatrix. In the core $T_e/T_i > 1$
whilst this ratio reverses in the edge and SOL. To slightly offset the numerical cost of the computations, run on Tier-0 Joliot-Curie at GENCI@CEA and MareNostrum at Barcelona Supercomputing Center, we assume a reduced magnetic field on axis: \( B_0 = 1.7\text{T} \), which amounts to computing a plasma column of slightly smaller size \( \rho_*=1/300 \) on a \( 1/4 \) wedge torus with \( (r,\theta,\varphi,v_\parallel,\mu)=(512,1024,64,128,64) \) grid.

Extensive tests have been performed to assess the robustness of the reported main results: observed gradient anisotropy and magnitudes in the limited configuration are robust whilst varying distribution function initialisation (local or canonical Maxwellians), presheath values in the SOL through \( \Lambda \) scans (from 0 to 5, its nominal value for Deuterium being \( \Lambda \sim 4.1 \)), target penalised temperature \( T_w \) in the limiter and wall, limiter shape (large and flat, narrow, rounded) and poloidal location (bottom, top). Further scans have also been performed in a flux-driven poloidally symmetric setting akin to Case-2, varying the \( T_e/T_i \) ratio, changing the safety factor \( q \) and magnetic shear \( s \) and altering the experimental density gradient. The latter two are illustrated in Fig.\ref{A-2}. Of course, details of edge transport vary with the various parameters scanned. Precise discussion of sensitivity is not within the scope of the current manuscript; the bottomline conclusion is that the reported dynamics of Case-1 (modified outer edge linear stability, nonlinear destabilisation and ensuing transport barrier onset) requires the combined possibility for plasma-boundary interplay and turbulence spreading. Absence of one or both prevents as in Cases-2 and 3 transport barrier onset and leads to transport shortfalls in NMsL of varying severity.

**Linear stability analysis** – of the poloidally-symmetric and limited GYSELA profiles is performed using the initial value framework of the Gyrokinetic Workshop (GKW) code \cite{14}, based on the gradient-driven and local (flux-tube) approximations. Unless stated otherwise (see Strategy III below) Boltzmann electrons have been assumed, as in Gysela. Growth rates for the most unstable poloidal wavenumbers \( k_\theta \rho_i = 0.6 \) in the poloidally-symmetric (Fig.\ref{A-3}) and limited (Fig.\ref{A-4}) configurations are estimated by the following procedure.

(i) at a given radial location \( r_0 \), compute the set \( \Sigma_{r_0} = \{q,s,\nu_*,T_i/T_e,U',\gamma_E,R/L_T,R/L_n\} \) of local values of the GYSELA plasma parameters, \( q \) being the safety factor, \( s = (r/q)dq/dr \) the magnetic shear, \( \nu_* \) is the collisionality, \( U' \) the parallel flow shear, \( \gamma_E \) denotes the \( \mathbf{E} \times \mathbf{B} \) shear, \( R \) the tokamak major radius and \( L_X^{-1} = -d(\text{Log}X)/dr \) with \( X = \{T,n\} \) the local logarithmic
Fig. A-2. Series of flux-driven computations at $\rho_\ast = 1/316$, akin to Case-2 but for the outer boundary conditions. In lieu of the penalised poloidally symmetric SOL of Case-2, an outer diffusive buffer region between $1 \leq r/a \leq 1.3$ surrounds the confined plasmas through application of the diffusion operator $D$ in Eq. (A-2), detailed as Eq.(50) in [4]. The goal is twofold: assess sensitivity (beyond experimental uncertainties) of edge transport dynamics to variations or uncertainties in input profiles and evaluate incidence of surrounding artificial diffusion for edge transport. Density gradients have a stabilising effect on the dominant Ion temperature Gradient (ITG) instability. Subplots (a) and (b) display incremental relaxation of density gradients past $r/a \geq 0.6$ and their incidence on fluctuation levels. Similarly, lower magnetic shear and safety factor values past $r/a \geq 0.6$ modestly increase fluctuations there. In all cases, edge fluctuation levels are lower than in comparable Case-2. In the absence of outer edge turbulent activity, core to edge spreading appears subdominant. Technically, the choice of an outer diffusive boundary region, though efficient numerically is thus not innocuous (and probably quite poor) on physical grounds. Interestingly also, despite large variations (beyond experimental uncertainties) of the mean density and safety factor profiles, the shortfall problem still exists despite large variations of the mean density and safety factor profiles, another indication that transport in the edge may not readily be understood on local and linear grounds alone.
Fig. A-3. Data from flux-driven poloidally-symmetric Case-2, at equilibrium ($t \Omega_{ci} = 200,000$). (a) Poloidal cross-section snapshot of the fluctuating electric potential. Specific locations are marked, combination of three radial locations: $\{r_1, r_2, r_3\}/a = \{0.90 \text{ (circles)}, 0.96 \text{ (stars)}, 1.02 \text{ (squares)}\}$ and four poloidal locations $\theta_k = \{9^\circ \text{ (magenta)}, 126^\circ \text{ (cyan)}, -118^\circ \text{ (red)}, -61^\circ \text{ (yellow)}\}$. Properties at these locations are shown in subplots (b): $E \times B$ shear, (c): parallel velocity shear and (d) through (f): maximal linear instability growth rate at vanishing $E \times B$ shear, keeping the same symbol–color combination.

Gradients of respectively ion temperature and density;

(ii) within GKW, the local approximation requires mean gradients to be constant over the computational domain, the numerical representation of a flux tube. Coarse-graining of the flux-driven GYSELA values is thus performed over a typical radial turbulence length scale $\Delta r = 10\rho_i$ and in time over the observed linear growth $\Delta t \Omega_{ci} = 25 \times 10^3$ of turbulent fluctuations. Furthermore, as the computational domain of GKW winds around the torus parsing both poloidal and toroidal angles, the background state is assumed to be uniform. This implies poloidal homogeneity along the flux tube and requires further averaging the GYSELA values on a flux-surface $(\theta, \phi)$: $\langle \langle \langle \langle \Sigma_{r_0} \rangle \Delta t \rangle \Delta r \rangle \theta \rangle \phi$, where $\langle \cdot \rangle_\zeta$ denotes the average over $\zeta$. Physically, it amounts to estimating...
Fig. A.4. Same layout as in Fig. A-3. Data is from flux-driven Case-1 with limiter at two different times: subplots (a) through (f) are early in the nonlinear development of turbulence \( t \Omega_{ci} = 30,000 \); subplots (g) through (l) at thermal equilibrium \( t \Omega_{ci} = 250,000 \). An additional location near the limiter at \( r/a = 0.96, \theta = -75^\circ \), marked by the large white triangle is shown and corresponds to the region of maximum linear instability growth.

the instability drive as if located at its ballooning angle, effectively maximising it;

(iii) for a chosen radial location \( r_j \), knowing \( \langle \langle \langle \Sigma_{r_j} \rangle \Delta r \rangle \Delta r \rangle \rangle \_\phi \) allows to compute with Gkw 2-dimensional maps of instability growth rates \( \gamma_{lin} \) as a function of the logarithmic gradients [subplots Fig. A-3 (d) to (f) and Fig. A-4 (d) to (f) and (j) to (l)], each map tailored to the precise
background local values in GYSELA for $T_i/T_e$, etc. Importantly, these maps are estimated at vanishing $E \times B$ shear;

(iv) we now estimate local values of the GYSELA local growth rates $\gamma_{\text{lin}}$ at 13 different radial-poloidal $(r_j, \theta_k)$ locations (shown in Fig.1 as well), combination of three radial locations near the separatrix: \{r_1, r_2, r_3\}/a = \{0.90 \text{ (circles)}, 0.96 \text{ (stars)}, 1.02 \text{ (squares)}\} and five poloidal locations $\theta_k = \{9^\circ, 126^\circ, -118^\circ, -75^\circ, -61^\circ\}$, spanning the full poloidal cross-section;

(v) in order to assess actual stability, one can estimate an effective linear growth rate correcting for the $E \times B$ shear: $\gamma_{\text{eff}} = \gamma_{\text{lin}} - \gamma_E$ [strategy I] or run Gkw nonlinearly, including $\gamma_E$ from GYSELA [strategy II]. This latter strategy is significantly more demanding numerically and only a few cases have been investigated. Furthermore, 2 additional runs with Gkw have been performed at \((r/a = 0.84, \theta = 9^\circ)\) and \((r/a = 0.96, \theta = 9^\circ)\) with a fully kinetic electron response to assess the impact of the Boltzmann electron approximation [strategy III].

For all Cases, the dominant instabilities inside $r/a \leq 0.84$ are found to be of interchange character. With a Boltzmann electron response, the ion temperature gradient (ITG) is dominant. With a kinetic electron response the instability inside $r/a \leq 0.84$ is a combination of ITG and Trapped electron modes (TEM).

- In poloidally-symmetric Cases-2 and 3, Gkw finds the edge to be marginally stable at vanishing $E \times B$ shear: $\gamma_{\text{lin}} \approx 0$ [Fig.4A-3-(d) to (f)]. When including $E \times B$ shear, strategy I predicts the edge to be nonlinearly unconditionally stable past $r/a \geq 0.9$, with $\gamma_{\text{eff}} < 0$ for all radial–poloidal combinations considered. Strategies II and III confirm that location \((r/a = 0.96, \theta = 9^\circ)\) is indeed stable. Contributions of perpendicular and parallel shear flow (parallel velocity gradient, PVG) instability \cite{15} are weak [Fig.4A-3-(c)] and insufficient to destabilise NMsL.

- In Case-1 with limiter the situation dramatically changes: destabilisation of the outer edge starts about the limiter, just inside the separatrix. Fig.4A-4-(e) shows estimated ITG growth rates at $r/a = 0.96$ that are larger than in Cases-2 and 3 whilst all locations at $r/a = 0.9$ remain stable [Fig.4A-4-(a) and (d)]. Effective growth rates are large in the vicinity of the limiter at locations $\theta = -75^\circ$ and $-61^\circ$. Instability growth is also predicted at the plasma top $\theta = 126^\circ$. 
Interestingly, as the limiter remains a cold sink throughout nonlinear regime, the near-limiter drive endures [Fig.A-4-(k)] and as turbulence spreads, formerly stable regions are destabilised [Fig.A-4-(g) and (j)]. Both $E \times B$ shear [Figs.A-4-(b) and (h)] and parallel velocity gradient [Figs.A-4-(c) and (i)] are significantly increased with respect to poloidally-symmetric Cases-2 and 3. The significant velocity shear near the separatrix is found to contribute a modest albeit positive fraction of the global instability with $\gamma_{PVG} \equiv |M_{||}L_{n||}^{-1} - L_{n}^{-1}| \approx 0$, when averaged on a flux surface. Here $M_{||}$ is the parallel Mach number. Local values however of parallel velocity shear about the limiter may locally reach up to 3 to 5 times the mean with $\gamma_{PVG} \gtrsim 0$, which does not rule out the possibility for localised yet significant free energy sources from parallel shear flow instability.

It is important to note that even though this procedure provides information on the nature of instabilities at play, two major and oft-made approximations in local approaches should be relaxed to accurately interpret flux-driven dynamics near the separatrix. Indeed, the local $E \times B$ shearing rates obtained from limited Gysela with respect to poloidally-symmetric cases [respectively comparing Figs.A-4-(b) and (h) to Fig.A-3-(b)] are large enough to significantly decrease linear growth, as currently estimated through $GKW$. Strategy I balancing maximum growth with $E \times B$ shear only provides partial insight into the nature of active instabilities. Secondly, postulating poloidal (parallel) homogeneity as flux tubes wind around the torus is reasonably accurate in the core but clearly less justifiable to describe the near-separatrix in flux-driven limited configurations. Much of the nonlinear destabilisation of linearly stable edge is consequence of the onset of such poloidal inhomogeneities. Furthermore, additional stabilisation mechanisms are possible, such as profile coupling or poloidal shift of the envelope mode. This linear analysis thus likely provides an upper-bound estimate of the actual flux-driven instability growth. It has the merits however to confirm that the edge under poloidally-symmetric boundary conditions is linearly stable and that it gets destabilised locally in the vicinity of the cold sink, emphasising the central role of turbulence spreading in understanding global equilibration of the turbulence dynamics.

**Causal inference.** Causality detection in information theory is actively debated [16]. The “Transfer Entropy” ($TE$) method is a simple nonlinear extension of the Granger causality [17], introduced
by Schreiber [18] and investigated in magnetised plasmas by Van Milligen et al. [19]. The idea behind \( TE \) is simple: let’s consider a time series \( (x_i) \) of realisations of observable \( X \), with \( 0 \leq i \leq n \). If one can better predict its next realisation \( x_{n+1} \) using additional data from another time series \( (y_j) \) of observable \( Y \) with \( 0 \leq j \leq n \), then “\( Y \) transfers information (i.e. causes) \( X \)”, or more accurately as “\( Y \) forecasts \( X \)”, which constitutes the definition of causality here. This idea is quantified measuring deviation of transition probabilities from independence, i.e. from a stationary Markov process. In its simplest expression, if processes \( X \) and \( Y \) are independent, then the following generalised Markov property holds for all \( 0 \leq k \leq n \):

\[
p(x_{n+1}|x_{n-k},y_{n-k}) = p(x_{n+1}|x_{n-k})
\]

The standard notation for conditional probabilities is used here: \( p(a|b) \) is the probability of \( a \) knowing \( b \). If now processes \( X \) and \( Y \) are not independent, the ratio of these two transition probabilities provides a measure of how much information they may share. In other words, how much knowing values within \( Y \) in addition to past values in \( X \) may help to better evaluate next-step \( x_{n+1} \). This idea leads to the following definition of the Transfer Entropy (\( TE \)) from process \( Y \) to process \( X \):

\[
TE_{Y \rightarrow X}(k) = \sum p(x_{n+1},x_{n-k},y_{n-k}) \log \left( \frac{p(x_{n+1}|x_{n-k},y_{n-k})p(x_{n-k})}{p(x_{n+1}|x_{n-k})} \right)
\] (A-6)

where \( k \) is thus a time lag and represents the \( k \)-past of times series \( X \) and \( Y \). The summation process is detailed below, in Eq. (A-8). \( TE \) can equivalently be recast as a conditional mutual information and represents the additional amount of information that must be added to adequately represent the studied process \( p(x_{n+1}|x_{n-k},y_{n-k}) \) with respect to its reference Markov process \( p(x_{n+1}|x_{n-k}) \). In the absence of information flow from \( Y \) to \( X \), the logarithm vanishes as state \( Y \) has no influence on the transition probabilities of \( X \). It also follows that \( TE \) is directional, i.e. \( TE_{Y \rightarrow X} \neq TE_{X \rightarrow Y} \), effectively allowing to infer causality between processes \( X \) and \( Y \). \( TE \) displays interesting properties: it is independent of the relative magnitudes of signals \( X \) and \( Y \); it may apply to either linear and nonlinear regimes; it is easy to evaluate directly in real space rather than in Fourier space and is typically less demanding in terms of statistics than bispectral techniques. Practically, \( TE \) is evaluated expressing the conditional probabilities as joint probabilities \( p(x_{n+1}|x_{n-k},y_{n-k}) = p(x_{n+1},x_{n-k},y_{n-k})/p(x_{n-k},y_{n-k}) \) and computing the 4 multidimensional probability density functions (pdfs):

\[
TE_{Y \rightarrow X,\alpha}(k) = \sum p^\alpha(x_{n+1},x_{n-k},y_{n-k}) \log^\alpha \left( \frac{p(x_{n+1},x_{n-k},y_{n-k})p(x_{n-k})}{p(x_{n+1},x_{n-k})p(x_{n-k},y_{n-k})} \right)
\] (A-7)
as a function of time delay $k$ and normalised such that $0 \leq TE \leq 1$. The 4 pdfs in Eq. (A-7) result from a binning process of times series $X$ and $Y$, such that Eq. (A-7) is estimated in practice as:

$$TE_{Y \rightarrow X, \alpha}(k) = \sum_{i=1}^{\beta} \sum_{j=1}^{\beta} \sum_{l=1}^{\beta} \left[ p^{3d}(i,j,l) \right] \alpha \log \left( \frac{p^{3d}(i,j,l) p^{1d}(j)}{p^{2d}(i,j) p^{2d}(j,l)} \right)$$

(A-8)

where $p^{3d}, p^{2d}, p^{2d}_{xx}$ and $p^{1d}$ are the discretised versions of respectively $p(x_{n+1}, x_{n-k}, y_{n-k}), p(x_{n+1}, x_{n-k}), p(x_n-k, y_{n-k})$ and $p(x_{n-k})$. In order to have sufficient statistics, a bin size $\beta = 2$ or $\beta = 3$ is typically chosen, depending on the available length of the time series (the longer the times series, the larger $\beta$ can be). We introduced here the additional exponent $\alpha \geq 1$, which effectively represents a nonlinear threshold: low probabilities will be further reduced and higher ones amplified. In a complex setting, information may flow both ways, from $Y$ to $X$ and inversely. It is thus especially useful to define the net transfer entropy $\Delta_{X,Y}(TE)[k] = TE_{Y \rightarrow X}[k] - TE_{X \rightarrow Y}[k]$, which provides the net flow of information between processes $X$ and $Y$, at timelag $k$. In the manuscript, pdfs in Eq. (A-7) are discretised using $\beta^d = 2^d$ bins, with $d$ the dimensionality of the pdf. The nonlinear threshold exponent $\alpha$ is set to unity and $X$ and $Y$ are discretised at the same rate and enter the $TE$ calculation with zero temporal mean. Further details may be found in Ref. [20].

We systematically apply the $TE$ algorithm to actual time series from the flux-driven Case-1 computation with limiter boundary conditions in the last 5% inside the separatrix, where the spontaneous onset of a persistent transport barrier is observed. The following vorticity equation [20–22] can be inferred from the primitive gyrokinetic equations including $E \times B$ drift and finite Larmor radius at leading order:

$$\partial_t \langle \Omega_r \rangle + \frac{1}{r} \partial_r \left[ \langle v_{Er} \Omega_r \rangle + \langle v_{*,r} \Omega_r \rangle - \left( \frac{v_{*, \theta}}{r} \partial_{\theta} E_r \right) \right] = r.h.s$$

$$r.h.s \approx -\partial_t \langle \Omega_\theta \rangle - \frac{1}{r} \partial_{\theta} \langle (v_{E\theta} + v_{*,\theta}) \Omega_\theta \rangle - \partial_r \frac{1}{2r} \partial_{\theta} \langle v_{E\theta}^2 \rangle + \frac{1}{2r^3} \partial_{\theta} \partial_r \langle r^2 v_{E\theta}^2 \rangle - \frac{1}{r} \partial_{\theta} \left( \frac{v_{*, \theta}}{r} \partial_{\theta} v_{E\theta} \right)$$

(A-9)

$$\Omega_r = \partial_r (r \partial_r \phi) / r \quad \& \quad \Omega_\theta = \partial_\theta^2 \phi / r^2$$

(A-10)

$$v_{Er} = -\partial_{\theta} \phi / r \quad \& \quad v_{E\theta} = \partial_r \phi = -E_r$$

(A-11)

$$v_{*,r} = -\partial_{\theta} p_{\perp} / r \quad \& \quad v_{*,\theta} = \partial_r p_{\perp}$$

(A-12)

where $\langle \cdot \rangle$ denotes an average over toroidal angle $\varphi$. The $TE$ algorithm is applied to many of the
possible permutations of quantities in Eq. (A-9) and especially here to the following set:

\[(X, Y) \in \left\{ \langle \Omega_r \rangle , \langle v_{Er} \Omega_r \rangle , \langle v_r \Omega_r \rangle , -\left( \frac{v_{r\theta}}{r} \partial_\theta E_r \right) \right\} \] (A-14)

Conclusions. – Methods described here have allowed to establish in Ref. [23] the following:

(i) Plasma—boundary interaction deeply modifies convective stability next to the magnetic separatrix;

(ii) Resulting locally-born eddies spread out and destabilise distant regions of the edge and core. A globally organised state emerges, ‘nonlocally’ [12, 13, 24] controlled by fluxes of turbulence activity;

(iii) Flow shear builds as eddies (vorticity) are advected, primarily through pressure inhomogeneities. The expanding interface organises into a stable peripheral transport barrier, i.e. into improved confinement.

This certainly stresses a key role for finite Larmor radius effects, i.e. for perpendicular pressure fluctuations. Though challenging, experimental measurements of such fluctuations and of their associated radially-inward, poloidally-anisotropic advections (spreading) could prove especially important to diagnose to deeply test our understanding of underlying mechanisms in the plasma edge, especially prior or at transport barrier inception.

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