The problem of capturing marginality in model reductions of turbulence

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Abstract
Reduced quasilinear and nonlinear (gradient-driven) models with scale separations, commonly used to interpret experiments and to forecast turbulent transport levels in magnetised plasmas, are tested against nonlinear models without scale separations (flux-driven). Two distinct regimes of turbulence—either above threshold or near marginal stability—are investigated with Boltzmann electrons. The success of reduced models hinges in particular on the reproduction of nonlinear fluxes. Good agreement between models is found above threshold, whilst reduced models significantly underpredict fluxes near marginality, overlooking mesoscale flow organisation and turbulence self-advection. Constructive prescriptions whereby to improve reduced models are discussed.

Keywords: turbulence, model reduction, self-organisation, marginality

1. Introduction
Fusion plasmas display the property, common in dynamical systems, that upon surpassing a critical threshold, an instability may promptly build up, inducing large fluxes that deplete the driving gradients and inhibit the instability. Background gradients thus hover in the vicinity of nonlinear near-marginal thresholds [1]. Many strategies have been devised in modelling to mimic natural processes. These are not all equivalent, and different choices may critically affect the nature of computed statistical equilibria.

Forcing-dependent steady states have indeed long been observed in a variety of systems. Systems with long-range interactions, either controlled in energy or in temperature, display different equilibria [2, 3]. Swirling flows controlled through either an imposed torque or an imposed velocity display distinct steady states, as well as different dynamical regimes [4]. In magnetised fusion plasmas, auxiliary heating and current drive force the system out of equilibrium through a constant flux. Mimicking nature, ’flux-driven’ (FD) forcing adiabatically imparts a volumetric flux to the system, whose gradients self-consistently adapt, leading to the observation of large-scale transport events such as avalanches [5–11], secondary nonlinear structures such as zonal mean flows [12, 13], or tertiary patterns such as staircases [14–19]. Such observations are absent or impaired when the system is driven through a body force, which amounts to imposing fixed mean gradients. This ’gradient-driven’ (GD) strategy is widely used in direct numerical computations as it is computationally efficient. It indeed enforces, with respect to the FD approach, spatial and temporal scale separations between equilibrium and fluctuations and solves for the fluctuations only.
Known differences between FD and GD frameworks have been documented [17, 18, 20], and related aspects have been discussed in several reviews [21–23]. Whether these are of practical incidence in fusion-relevant configurations is nontrivial, and these questions are likely exacerbated in near-marginal regimes. This matter is important because there are increasing requirements for fast, reduced, yet reliable models to explore the vast parameter space of magnetised plasma turbulence, interpret experimental results and forecast future large experiments such as ITER. Currently, the more advanced reduced models are based on quasi-linear (QL) theory (QLT) [24–26]. With the advent of machine learning techniques, the ubiquitous closure problem of QLT is approached through data-driven techniques that use large-scale databases of gyrokinetic GD computations. Systematic shortcomings, if any, within these reference GD strategies, are thus likely to be carried over to the reduced models. A comprehensive understanding of discrepancies between first-principles FD, GD and QL approaches is thus important and timely, and is the topic of this manuscript.

To this end, we confront reference results from nonlinear FD gyrokinetics using the Gysela framework [27] to state-of-the-art GD nonlinear gyrokinetics and GD QL calculations, using respectively Gkw [28] and QuaLiKiz [29, 30]. We further complement the study with a twofold confrontation with the QL transport framework of QuaLiKiz–Jetto and with the nonlinear local transport framework of Gene–Tango. In these computations, \( N_{r,\text{eval}} \) instances of QuaLiKiz or Gene [31] locally compute at various radii \( r_{\text{eval},i} \) (with \( 0 \leq i \leq N_{r,\text{eval}} \)) flux-surface-averaged transport coefficients, which are passed on to the Jetto [32] or Tango [33] one-dimensional integrated modelling suites and used to evolve profiles through FD transport equations. After a transport time scale, new local values at each \( r_{\text{eval},i} \) location from the evolved profiles are fed to local QuaLiKiz or Gene and the process loops. In practice, \( N_{r,\text{eval}} = 50 \) for QuaLiKiz–Jetto and \( N_{r,\text{eval}} = 9 \) for Gene–Tango.

Our main results are: (i) steady-state predictions of fluxes moderately depend on the nature of forcing well above the nonlinear threshold; (ii) near marginality, however, nonlinear and QL GD models sizeably underpredict turbulent heat transport. Under a driving flux, profiles display ‘stiffness’, i.e., they hover in the vicinity of their near-threshold flux-matching values. Large, hot devices, such as ITER, are expected to be stiff due to the temperature dependence of the gyroBohm heat flux scaling, making near-marginality a regime that models must confront. Proximity to nonlinear thresholds implies additional complexity as it favours secondary pattern formation and mesoscale organisation. Despite this additional complexity, (iii) the underlying assumptions of QLT hold well across nonlinear regimes. We show that transport underprediction rather stems from the choice of closure, i.e. the nonlinear saturation rule. This work stresses the relevance of QLT for model reductions of turbulence whilst providing guidelines whereby reduced models can be improved. The nonlinear and QL approaches tested here are the current workhorse for estimating transport and confinement in turbulent fusion plasmas. This work thus has implications for present-day experimental data analysis and scenario extrapolation for fusion production. Novel saturation rules should strive to incorporate near-marginal FD specificities, often dubbed turbulence spreading [11, 34–38], transport nonlocality or staircase organisation.

2. Frameworks compared

Models are often categorised on being either ‘local’ (e.g. ‘flux-tube’) or ‘global’. In the local approximation, mean profiles are piecewise constant and boundary conditions periodic; in the global approach, both assumptions are relaxed. There are documented differences between both approaches, but for the present discussion, being either local or global is secondary to the fact of being either GD or FD. Large-scale mean (equilibrium) gradients, as the main source of free energy, will of course contribute to driving meso- and microscale dynamics. Micro- and mesoscales back react nonlinearly on the equilibrium profiles via turbulent fluxes. A central question is whether any scale separation (in time and space) exists between turbulence dynamics at the micro- and mesoscales, on the one hand, and equilibrium scales, on the other hand. This question is likely all the more critical close to (nonlinear) marginal stability, where mesoscale dynamics are more pronounced, with the memory of smaller scale turbulent activity being ‘stored’ in mesoscale alteration of equilibrium profiles.

Importantly, in FD frameworks, no scale separation between equilibrium and fluctuations is postulated, which implies that the sources and sinks that drive the system out of equilibrium evolve on length scales coarser than that of the turbulence as well as on slow, adiabatic time scales. A continuum of (turbulent) micro- and mesoscales can thus be fed back to meso- to macroscales. In this respect, FD approaches are necessarily global whilst the inverse is not true. One could thus argue that FD and global GD approaches should render close results well above threshold. Closer to the (nonlinear) turbulence threshold, near-marginal regimes are precisely the regimes where global GD approaches may prove significantly different from FD approaches, for instance through manifestation of self-organised criticality-like phenomena. The curious reader is also referred to e.g. section 4 of [21], which further illustrates these matters.

FD Gysela resolves ion Larmor radius scale turbulence and collisional transport in the global tokamak geometry, spanning from \( r/a = 0 \) to \( r/a = 1.2, a \) being the minor radius of the torus. A centrally peaked heat source drives a deuterium plasma out of equilibrium. For \( r/a \geq 1 \), a heat sink is progressively applied, which allows convergence to a steady temperature profile on energy confinement times. The steady-state and coarse-grained (see below) density \( n \), temperature \( T \), source \( S \) and safety factor \( q \) profiles from Gysela are shown in figure 1. Together with the zonal mean shear shown in figure 2, they are the reference inputs used to initialise all the other codes. On
practical grounds, the GYSELA profiles require some amount of coarse graining or smoothing before serving as input for either GKW or QUALIKIZ: this is the essence of the scale separation assumption inherent to the GD approach. In a GD framework and even more so in the local limit, profiles are indeed required to be smooth below a cut-off radial scale \( \ell \ll \ell_\ell = \max(\lambda_{\text{lin}}, \lambda_{E \times B}) \), whose physics are not included within GD models. Here \( \lambda_{\text{lin}} \gtrsim 10-20 \rho_i \) denotes the typical radial extent of unstable growing modes and \( \lambda_{E \times B} \gtrsim 10 \rho_i \) the typical width of mean \( E \times B \) shear structures [15]. To this end, GYSELA observables are both time-averaged at steady state over \( 30000 \Omega_i \rho_i \) —which is larger than a typical linear growth time and radially smoothed through sliding windows of \( 60 \rho_i \) to smear out FD specificities in the profiles. Here, \( \Omega_i \) is the ion cyclotron frequency. Sliding averages of \( 20 \rho_i \) have also been investigated and found insufficient near marginality to smear out memory of meso scale organisation from the FD framework. This point is further discussed below whilst evoking the role of mean \( E \times B \) shear.

GD models, on the other hand, (either local or global) exploit to numerical advantage the assumption of a scale separation between a fixed (mean) equilibrium and fluctuations. Sources and sinks are also required in GD approaches to maintain the system out of equilibrium; the important point is that they depend on the local dynamics of the plasma: maintaining fixed background mean gradients thus acts so as to counteract part of the natural dynamics of the system (which would naturally relax towards equilibrium), especially hindering spreading and mesoscale dynamics. The appealing semantic contrast between local and global may sometimes cloud the important fact that, especially near marginal stability, what matters is whether these scale separations are postulated or not. Said differently, models are better classified near marginal stability on whether scale separations are postulated or not, whether mesoscale organisation can develop or not and turbulence spreading can occur, unhindered. These questions have been documented both with Boltzmann and kinetic electron responses—see e.g. figure 2 in [16], figures 5 and 9 in [17], and figures 10 and 11 in [18, 39, 40]. The inclusion of electron dynamics bears additional physics that will be specifically addressed in an upcoming work. In the present manuscript, we compare as a first step all approaches with Boltzmann electrons.

GD nonlinear GKW exists in both local and global versions; it is here run in its local (flux-tube) setting, solving a limited subset of the whole plasma volume twisting around the torus due to the magnetic shear of the background magnetic equilibrium. GKW is compared to GYSELA at three different locations \( r/a = 0.3, 0.4 \) and 0.6. At each of these locations, one first computes the coarse-grained values of the GYSELA profiles (as detailed above) at equilibrium, shown in figures 1 and 2. These values are used to define the reference background Maxwellian for GKW at each location; GKW then evolves the perturbed distribution function with reference to this fixed background. The resolution chosen for all GKW runs is such that resolved radial and poloidal wavenumbers extend from \( (k_r \rho_i)_{\min} = (k_r \rho_i)_{\min} = 0.051 \) to \( (k_r \rho_i)_{\max} = 2.6 \) and \( (k_r \rho_i)_{\max} \) is adjusted to match the radial resolution used in GYSELA, i.e. 11.3 for the ‘above threshold’ case and 8.1 for the ‘near-marginal’ one. This amounts to a radial box size that spans \( 1/(k_r)_{\min} = 2 \pi \times 19.6 \rho_i \approx 120 \rho_i \) at the low field side midplane. Since the GKW computations, in consistency with the local framework are radially periodic, a large radial box size of \( \sim 120 \rho_i \) helps avoid unnatural interactions with the periodic boundaries. GKW thus effectively computes at each location \( r/a = 0.3, 0.4 \) and 0.6 a nonlinear realisation in the local GD approximation of the dynamics locally expected of the coarse-grained FD GYSELA profiles.

Further reducing the model complexity, turbulent structures are expected with the QL approximation to bear memory in the shape and localisation of their linear generation mechanism. They remain radially thin around a reference magnetic surface and only depend on local plasma parameters and local gradients. This is a direct consequence of the assumption that relates the distribution function fluctuations to the potential fluctuations through local equilibrium parameters. This induces, as with the GD approach, a spatial scale separation between the local turbulent behaviour, and a slower and smoother evolution of the profiles. Quasilinear QUALIKIZ is run here in two configurations: in its standalone version, it is inherently local; in its version coupled to the transport code JETTO, the local transport coefficients from QUALIKIZ are used as inputs for transport equations, thus allowing for the equilibrium to evolve on transport time scales whilst retaining the locality and scale separation assumptions on shorter length and time scales. QUALIKIZ solves the gyro-kinetic dispersion relation, here with Boltzmann electrons. For efficiency, the analytic distribution response is simplified by computing the shape of the potential fluctuations in the fluid limit [29], while keeping a kinetic treatment of the wave-particle resonance. Stable modes are neglected; unstable modes are accounted for through a double power law in \( k_\parallel \) for the turbulent intensity spectrum. The number of numerical integrations is limited by performing the resonant velocity integration analytically. The effect of zonal flow shear is modelled by perturbative modification of this response. Extensive benchmarks with local GD gyrokinetic codes have led to refining the closure for the potential
fluctuations [30, 41], calibrated to a database of local nonlinear gyrokinetic simulations akin to those presented here with Gkw.

Finally, two additional series of computations have been performed in the near-marginal and above threshold settings using the integrated scheme of Gene–Tango. This additional framework complements the Gkw and QuaLiKiz–Jetto approaches: Gene is a GD local nonlinear gyrokinetic framework akin to Gkw, and the transport framework of Tango is similar to Jetto. Comparison between the combined Gene–Tango and QuaLiKiz–Jetto frameworks allows us to test (i) the impact of the QL reduction with respect to nonlinear evolution. Since both Gene and QuaLiKiz have scale separations built into their framework, comparison of both approaches to GySELA also allows specific assessment of (ii) the influence of the scale separation assumption. This point is further discussed below and is found to be important near marginal stability.

All four approaches can handle complex geometries, but here, for the sake of simplicity, each is set to run in the same simplified toroidal magnetic geometry with circular and concentric flux surfaces $B = (B_0 R_0 / R) [r e_\theta / q R_0 + e_\phi]$, where $e_\theta$ and $e_\phi$ are the unit vectors in the poloidal and toroidal directions, $B_0$ is the magnetic field on axis, $r$ the minor radius and $R = R_0 + r \cos \theta$ the major radius.

Let us close this section with two concluding remarks. First, it is worth emphasising that the impact of the type of forcing on turbulent transport and achievable steady states is not restricted to numerical simulations. Experimentally, it is well documented in fluids that the statistics of flow states as well as transitions between them may critically depend on the type of forcing applied—e.g. in von Kármán flows either at constant impeller speed or at constant torque [4]. These observations are analogous to the GD and FD cases respectively discussed above. Not surprisingly, the difference between both regimes manifests close to transitions between two equilibrium states while disappearing away from the transition. Again, this behaviour is reminiscent of magnetised plasma dynamics near marginal (nonlinear) stability or above threshold.

Finally comes the important question of the nonlinear saturation of turbulence in all three approaches. $\mathbf{E} \times \mathbf{B}$ shear has at least two components, a mean part and a fluctuating part, which may affect and regulate the system differently, over different time scales and through possibly distinct pumping and damping mechanisms. In GySELA both components are self-consistently computed and act in concert. The radial force balance $E_r - V_T B_\phi + V_\phi B_r - \nabla p / ne$ is satisfied throughout the computation [42]. This is not so for QuaLiKiz, Gkw or Gene, for which the mean part is unconstrained. The input can be freely imposed in local approaches without breaking constitutive orderings, echoing the fact that the above radial force balance does not need to be satisfied. Gkw and Gene thus only compute the fluctuating $\mathbf{E} \times \mathbf{B}$ shear as part of the nonlinear response. For QuaLiKiz in its standalone version, the mean $\mathbf{E} \times \mathbf{B}$ shear is an input as well, and the effect of the fluctuating $\mathbf{E} \times \mathbf{B}$ flows on the saturation of turbulence is part of the closure scheme, thus approximated by local nonlinear gyrokinetics. In the QuaLiKiz–Jetto framework, this must be slightly nuanced: (i) the transport equation leads to an evolving pressure gradient; (ii) the toroidal velocity $V_T$ can either be prescribed from measurements or self-consistently from the momentum transport equation including the external torque and QuaLiKiz momentum transport, and (iii) the poloidal velocity $V_p$ is evaluated from the neoclassical transport model NCLASS [43]. The QuaLiKiz–Jetto interface then estimates $E_r$ through radial force balance. From there comes the perpendicular velocity shear input into QuaLiKiz at each radial grid point. Note that a similar procedure exists in the Gene–Tango interface but has not been used for the present study. Note as well that even with this consistent evaluation of radial force balance not all relevant flows are taken into account in these approaches and in particular no structuring at mesoscales can occur due to the built-in scale separation assumptions. In the case of QuaLiKiz there are also additional missing intrinsic rotation or turbulence-generated zonal flow effects.

In the present manuscript, we focus on testing the consequences of constitutive assumptions in the models and therefore choose to impose in Gkw and QuaLiKiz the local values of mean $\mathbf{E} \times \mathbf{B}$ shear from GySELA. One could also ask for a complementary approach and for example only consider the self-consistent fluctuating $\mathbf{E} \times \mathbf{B}$ shear from nonlinear Gkw or Gene, or the shear effectively allowed in QuaLiKiz through the choice of closure, and ask how this would compare to GySELA. This is done in the Gene–Tango framework where the mean $\mathbf{E} \times \mathbf{B}$ shear from GySELA is not imposed and only the fluctuating $\mathbf{E} \times \mathbf{B}$ shear from Gene is included. A comprehensive discussion of these issues is beyond the scope of the present work, but one would expect discrepancies between models to be especially visible near marginal stability. Indeed, the possibility to self-consistently evaluate the mean $\mathbf{E} \times \mathbf{B}$ shear is directly connected to the role of mesoscale organisation, and only fully present in FD GySELA. To illustrate this point, let us emphasise that the computed fluxes from Gkw and especially from QuaLiKiz show significant sensitivity near marginality to imposed levels of mean $\mathbf{E} \times \mathbf{B}$ shear (within one standard deviation) when the mean $\mathbf{E} \times \mathbf{B}$ shear profiles from GySELA are only smoothed over 20$\rho_i$ (approximately twice the mean flow width or the width of mean profile corrugations [18]). This sensitivity is much less pronounced with the 60$\rho_i$ radial smoothing of the GySELA profiles reported here. This is certainly illustrative of the important role that the mean $\mathbf{E} \times \mathbf{B}$ shear plays in FD approaches near marginality. Conversely, the fact that QuaLiKiz–Jetto and Gene–Tango provide comparable results with the 60$\rho_i$ radial smoothing, despite different imposed levels of mean $\mathbf{E} \times \mathbf{B}$, shows that the strong coarse graining applied to GySELA effectively minimises discrepancies with the other approaches. The near-marginal flux underprediction that we report below is thus likely significant and possibly a lower-bound estimate of the actual differences.

This question of a consistent evaluation of mean $\mathbf{E} \times \mathbf{B}$ shear/of mesoscale organisation is certainly an interesting one for prospective GD computations, which aim to provide
quantitative answers for new/untested plasma configurations for which there is no a priori ‘ground truth’ (experimental or FD). To try to mitigate this problem, local frameworks are increasingly coupled to transport equations, which provide a step towards a more self-consistent coupling between mean and fluctuations. In this respect, the lingering discrepancy between Gysela on the one hand and both QuaLiKiz–Jetto and Gene–Tango on the other hand, visible in figure 4(c), is certainly indicative of the fact that coupled models where the turbulence model is based on a scale separation still miss part of the dynamics near marginal stability. This important observation certainly calls for further studies on the matter, whilst especially relaxing the assumption of Boltzmann electrons.

3. Two distinct regimes

Two paradigmatic simulation regimes are considered in the electrostatic regime with Boltzmann electrons. Both cases are run in the so-called ‘local limit’ [44], at \( \rho_s = \rho_i/a \ll 1/250 \), where comparison to local Gkw is fair. The coarse-grained (see above) radial profiles of normalised temperature gradients \( R/L_T = -R_0 T/|T| \) and zonal flow shear are plotted in figure 2 for the above threshold (top) and nearmarginal (bottom) cases. The shaded areas represent temporal standard variations. The large deviation from the mean shearing rate in the near-marginal’case (bottom, right axis) results from the meandering of staircases, which have already been reported to play an important role in this regime of parameters [18]. The linear (black hourglass symbols) and nonlinear (red squares) thresholds are discussed in the next section. In order to broadly span parameter regimes, the main plasma parameters vary significantly between cases, as illustrated in table 1. This choice echoes the fact that the parameter space is broad, and parsing it is not easy. The comprehensive discussion of the precise impact of each parameter (\( \rho_s \), aspect ratio \( R/a \), \( \tau \) …) is a daunting task. We take a first step in this direction and choose to broadly span parameters from the near-marginal case to the above threshold case. One wishes thus to minimise the possibility that the found conclusions may strongly depend on the precise corner of parameter space that is investigated. Of course, the present approach will need to be complemented by further dedicated studies specifically focusing on scanning one parameter or the other.

Our choice of parameters in table 1 is, however, not totally random, as we have performed with Gysela extensive aspect ratio (in the range \( R/a = 3–10 \)) and \( \rho_s \) scans (in the range \( \rho_s^{-1} = 190–380 \)) and numerically found a confinement time scaling law of the form \( \tau \Omega_i \propto (R/a)^{0.88} \rho_s^{-2.4} \) [45]. The near-marginal case has both a larger \( \rho_s \) and a lower aspect ratio than the above threshold case. Given the above scaling, one may expect for the near-marginal case a degraded confinement with respect to what would have been obtained should we have run the near-marginal profiles with the \( R/a \) and \( \rho_s \) parameters of the above threshold case. This is an important point: the parameters chosen for the near-marginal case are not such that they strengthen FD specificities. Rather the opposite: beneficial zonal flow activity through the mesoscale staircase organisation is indeed observed to be enhanced at smaller \( \rho_s \) values [14], allowing the favourable gyro-Bohm-like confinement scaling to be recovered by taming the avalanching/spreading activity through successive staircase steps (see e.g. section 2.4 in [18]). Anticipating in the following sections the discrepancy found in the near-marginal regime between Gysela on the one hand and either Gkw, QuaLiKiz, QuaLiKiz–Jetto or Gene–Tango on the other hand strengthens the necessity to further understand and incorporate near-marginal physics in reduced GD or QL models of turbulence.

For each set of local values of the Gysela parameters, two thresholds are to be distinguished: linear \( R/L_T^{ie} \) represents the normalised temperature gradient, above which an unstable mode grows, at vanishing \( E \times B \) shear. The inclusion of self-generated flow shear—nonlinear in essence—introduces a
second threshold \( R/L_T \), indicative of the nonlinear saturation of turbulence [46], in particular by zonal flows. Practically, \( R/L_T \) is computed in local GD frameworks as the minimum local temperature gradient, which provides a non-vanishing nonlinear heat flux. It is estimated with Gkw through a series of increasing \( R/L_T \) nonlinear computations, whilst imposing local \( \mathbf{E} \times \mathbf{B} \) shear values from FD Gysela.

‘Above threshold’ is used to refer to regimes such as \( R/L_T^{\text{lin}} < R/L_T \), characterised by a static, smooth zonal mean shear \( \tau_E = \partial^2 \phi / \partial \mathbf{B} \) and subdominant zonal fluctuations. The flux-surface average of the electric potential is \( \langle \phi \rangle \), and \( \tilde{\phi} \) are its fluctuations. ‘Near-marginal’ is used to refer to regimes such as \( R/L_T^{\text{lin}} < R/L_T \). Proximity from below to \( R/L_T \) is a hallmark of near-marginality, featuring a well-defined staircase pattern of flows and associated temperature corrugations that meander within the time interval—hence the large shear deviation—and significant avalanching activity [18].

### 4. Kubo numbers of order unity

QLT is valid [47] in the low Kubo number limit. Kubo numbers \( K = \tau_{\text{jump}} / \tau_{\text{int}} < 1 \) are the ratio of a jumping time \( \tau_{\text{jump}} \) of particles from one turbulent eddy to the next over a nonlinear eddy-particle interaction time \( \tau_{\text{int}} \). Kubo numbers are estimated from the Gysela FD data in various ways, summarised in table 2. With analogy to incompressible fluids, particles trapped in turbulent convective cells explore eddies in a typical turnover time given by the local vorticity \( \tau_{\text{int}} \propto B / (\nabla \omega)^{1/2} \), whilst they undergo this vortical motion they also drift in about \( \tau_{\text{jump}} \propto L_0 (eB/\nabla T) \) from one turbulent structure to the next at the typical speed of the local diamagnetic velocity. Alternatively, the slower evolution of the potential field provides a relevant correlation time \( \tau_{\text{corr}} \) for turbulent fluctuations, a trade-off between unstable growth and nonlinear saturation. It must be computed as a Lagrangian correlation time in the co-moving frame of the eddies to correct for the Doppler shift due to the turbulence mean rotation and the eddy velocity. We estimate it through image registration, following the toroidal shift between three-dimensional turbulence snapshots of \( \phi \). It is compared to turbulence-driven stochastic transport times of particles, which, assuming a diffusive ansatz for \( \mathbf{E} \times \mathbf{B} \) fluctuations, drift across eddies in about \( \tau_{\text{diff},x} \propto L_x / (\nabla \phi_x)^{1/2} \), with \( x = \{ r, \theta \} \) and \( L_x \) the transverse correlation lengths computed from Gysela outputs. Interestingly, employing a Eulerian correlation time would result in severe Kubo number overestimation, locally up to factors of 25.

Three Kubo numbers, combinations of the above nonlinear times, are plotted in figure 3 for both above threshold and near-marginal regimes. The various definitions for \( K \) are coherent and provide the following picture: (i) on the basis of order unity Kubo numbers, QLT should be marginally valid. Yet, as shown below, key assumptions at the heart of the QLT reduction remain valid throughout nonlinear evolution, which strengthens the case for QL integrated modelling. Interestingly also, (ii) consistently larger \( K \) values near marginality stress the more percolative nature of transport there. Avalanching emerges as a key theme to distinguish between above threshold and near-marginal regimes as they likely underpin the larger \( K \) values computed near marginality. This is a likely indication that incorporating avalanching and its zonal mean flow regulation may significantly alter transport predictions and improve model behaviour near marginality.

### 5. Near-marginal heat flux underprediction

Heat fluxes are computed with QuaLiKiz, Gkw or Gne from the Gysela time-averaged steady-state profiles plotted in figures 1 and 2 with the same degree of approximation (electric and Boltzmann electrons). All codes have different normalisations, with Gysela for example being normalised to \( Q_y = Q/(n_i T_v v_{th}) \) with \( v_{th} = (T_v / m_i)^{1/2} \) the ion thermal velocity. In figures 4(a) and (b), fluxes from all codes are in units of \( Q = Q_y / Q_{y,\text{ion}} \), with \( Q_{y,\text{ion}} = \rho_s a / R \) and values of \( \rho_s, 50 \) and \( R/a \) given in table 1. Consistent rescaling factors have been applied to QuaLiKiz and Gkw fluxes. The non-axisymmetric (turbulent) contributions to heat fluxes are shown in figures 4(a) and (b). Turbulence spreading and profile corrugations, inherent to FD complexity, are absent or hindered in all QL and GD approaches. A fair comparison thus requests that the Gysela reference data be significantly coarse-grained before being handed over to Gkw, Gene or QuaLiKiz as input profiles. This smoothing includes the

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**Table 2.** Five typical wave–particle and turbulent times lead to three Kubo number combinations, shown in figure 3.

| Particle trapping \( \tau_{\text{jump}} \) | Transverse drifts \( \tau_{\text{diff}} \) | Eddy turnover \( \tau_{\text{int}} \) |
|-----------------------------------------|----------------------------------|-----------------------------|
| Random walks \( K^{(r,\theta)} \) | Lagrangian correlation time \( \tau_{\text{corr}} \) | \( \mathbf{E} \times \mathbf{B} \) random walk \( \tau_{\text{jump}}^{(r,\theta)} \) |

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**Figure 3.** Kubo numbers for the principal nonlinear dynamics in the problem. Plain and plusses: turbulent radial and poloidal \( \mathbf{E} \times \mathbf{B} \) velocity effect during a turbulent auto-correlation time. Circles: trapping of particles due to turbulent vorticity during transverse crossing of the turbulent filament.
is thus clearly questioned near marginality. Observations casting concern on near-marginal GD predictions of the observed large flux underprediction. This echoes previous bars. Secular growth of zonal flows in outside the allowed gradient sensitivity and fluctuation ‘error’ hierarchy. Conversely, near marginality, agreement in the computed fluxes is found across the fidelity (subplot (c)). In the regime above threshold, driven by a central source that mimics that of shear is mitigated when called within the integrated framework, whilst by factors in heat fluxes from one radial position to the next, LiKiz is responsible for in heat fluxes from one radial position to the next, LiKiz and despite the inclusion of shear, as detailed above, to smear out visible FD specificities in the profiles. The stabilising effect of mean zonal flow shear is accounted for in Gkw and QualiKiz whilst locally imposing the smoothed reference Gysela mean shear values. In Gene–Tango only the fluctuating $E \times B$ shear is included—see discussion above. Sensitivity to gradient fluctuations, inherent to GD approaches, is further assessed by additional scans in $R/L_T$ and $E \times B$ shear within one temporal standard deviation of the Gysela profiles.

Without inclusion of $E \times B$ shear stabilisation, [i] the QualiKiz heat fluxes are overestimated with respect to figure 4 by over an order of magnitude (not shown here). With the inclusion of shear, [ii] at locations of low or vanishing $E \times B$ shear and despite the $60\rho_i$ smoothing, GD (standalone) QualiKiz commonly displays (subplots (a) and (b)) variations by factors in heat fluxes from one radial position to the next, whilst Gkw exhibits much less sensitivity to $E \times B$ shear stabilisation. Interestingly, this large sensitivity of QualiKiz to shear is mitigated when called within the integrated framework of Jetto [32] to allow for an FD QL profile evolution, driven by a central source that mimics that of Gysela (subplot (c)). In the regime above threshold [iii], reasonable agreement in the computed fluxes is found across the fidelity hierarchy. Conversely, near marginality, [iv] despite significant smoothing, heat flux discrepancies in figure 4(b) are well outside the allowed gradient sensitivity and fluctuation ‘error’ bars. Secular growth of zonal flows in Gkw is responsible for the observed large flux underprediction. This echoes previous observations casting concern on near-marginal GD predictions [17]. The soundness of separating fluctuations from the mean is thus clearly questioned near marginality.

The conclusions above are further confirmed when comparing FD Gysela to the FD QL frameworks of QualiKiz–Jetto and Gene–Tango, in the same two regimes. In subplot (c), profiles from QualiKiz–Jetto and Gene–Tango are evolved until the heat fluxes match the nonlinear Gysela reference fluxes. The figure of merit now becomes how closely evolved the QL or nonlinear profiles are at flux equilibrium with those of Gysela. A remarkable [v] profile agreement is found for both approaches in the above threshold case, which in the case of QualiKiz also echoes the agreement in fluxes displayed in panel (a). Near marginality, however, [vi] a large overprediction of the temperature is required for both QualiKiz–Jetto and Gene–Tango to carry the same flux as Gysela. Interestingly, the fact that both QL QualiKiz–Jetto and nonlinear Gene–Tango frameworks provide consistent results illustrates the fact that [vii] the QL reduction is not a priori responsible for the observed flux under-prediction in the near-marginal regime. A constitutive ingredient is missing in this regime, at least with Boltzmann electrons, which is due to either the local or the GD approximation. This rather clearly [viii] points towards a problem with the scale separation assumption near marginality and gives a workable route for improvement.

6. Axis for improvement: saturation rules

Flux discrepancies between Gysela and Gkw likely stem from disregarding the feedback of fluctuations on an assumed fixed ‘equilibrium’. This enforces local and single-valued flux–gradient relations, and underestimates turbulence spreading, avalanching and mesoscale organisation. All of these contribute to transport, especially near marginality.

Figure 4. (a), (b) Gradient-driven QualiKiz and Gkw heat fluxes compared to reference flux-driven Gysela flux levels, based on the Gysela profiles of figure 2 and expressed in gyro-Bohm units. Grey shaded areas represent a standard deviation of Gysela heat fluxes during the considered time interval, as profiles fluctuate. Red and blue shaded areas represent the sensitivity of QualiKiz to these profile variations; the hourglass symbols that of Gkw to increased input temperature gradients. The reverse approach is followed in panel (c): heat fluxes in QualiKiz–Jetto and Gene–Tango are made to match the Gysela reference fluxes; the unknowns are thus the QualiKiz–Jetto and Gene–Tango profiles. The remarkable agreement above threshold and large overprediction of the temperature gradient near marginality are consistent with results in panels (a) and (b). This emphasises model reduction adequacy in above threshold regimes and missing physical ingredients in near-marginal regimes.

$E \times B$ shear profiles. Hence, time averaging over $30000\Omega_{ci}$ and radial smoothing over $60\rho_i$ are performed on the Gysela observables, as detailed above, to smear out visible FD specificities in the profiles. The stabilising effect of mean zonal flow shear is accounted for in Gkw and QualiKiz whilst locally imposing the smoothed reference Gysela mean shear values. In Gene–Tango only the fluctuating $E \times B$ shear is included—see discussion above. Sensitivity to gradient fluctuations, inherent to GD approaches, is further assessed by additional scans in $R/L_T$ and $E \times B$ shear within one temporal standard deviation of the Gysela profiles.

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Discrepancies with QuaLiKiz may either come from violating assumptions central to QLT—linearity of fluctuations—or by inheriting shortcomings akin to those of Gkw, through the choice of saturation rules.

To disentangle these questions, we compute in figure 5, for all three approaches, the complex argument \( \alpha_n \) of the \( n \)th Fourier component of the heat flux (panel (a))—a proxy for the linear cross-phase between the electric potential and pressure fluctuations. They depend on the toroidal wave number \( n \) labelling each eigenmode, which is related to the normalised poloidal wave vector \( k_\theta \rho_i \) through \( k_\theta \rho_i = (a/r)nq\rho_s \).

In the present cases, the \( n = 25 \) toroidal wave number corresponds to, at mid-radius \( a/r = 2; k_\theta \rho_i = 25 \times 1.4 \times 2/250 = 0.28 \) and \( k_\theta \rho_i = 25 \times 1.7 \times 2/350 \approx 0.24 \) for the near-marginal and above threshold cases, respectively. In Gysela, \( Q_{\text{sys}}^{\text{Gys}} \) is the squared potential \( |Q_n| \) of the Fourier components of the heat flux and of the squared potential \( |\phi_n|^2 \), i.e. the saturation rule, are respectively shown in panels (c) and (d). Panel (b) displays their ratio, a proxy for the dispersion relation, sometimes called ‘QL flux integrals’.

Clearly, linear cross-phases display reasonable agreement, within factors of 2 and across all regimes. They are not responsible for the flux discrepancies. Factors of disagreement—and avenues of improvement for QL modelling—are essentially twofold: [i] 90% of the heat flux is carried by modes \( n \in [5, 50] \) in the above threshold regime; all approaches provide similar conclusions. Near marginality, however, flux is carried in Gysela and Gkw through \( n \in [5, 70] \), twice the amount of active modes with respect to QuaLiKiz. Furthermore, [ii] saturation rules are clearly responsible for many of the observed flux discrepancies. In the above threshold regime, the flux spectra agree well (panel (c))—though this results from a surprising compensation: the potential, or saturation rule (panel (d)), is underestimated, and the dispersion relation (panel (b)) is overestimated, yet the heat flux spectra in the above threshold regime are in reasonable agreement. No such compensation occurs near marginality; there, severe underestimation of the potential spectrum is clearly responsible for the under-prediction of fluxes.

7. Outlook

The success of the reduced models hinges in particular on the reproduction of nonlinear gyrokinetic fluxes [30]. Flux underprediction in the dynamically important regime of near-marginal stability is thus a matter of importance. At the heart of this paper lies the fact that FD and GD models provide significantly different flux predictions with Boltzmann electrons close to marginal stability \( R/L_T \), which underpins basic discrepancies in how nonlinear saturation of turbulence is modelled. This should foster renewed interest in ways to complete QL or GD models near marginality. The robustness of linear features [48] across the fidelity hierarchy and across turbulent regimes is encouraging, and provides constructive directions whereby reduced models can be improved.

Discrepancies between the nonlinear frameworks of Gysela and of both Gkw and Gene–Tango are strong indications that turbulence spreading and mesoscale patterning are in fact central to accurate transport predictions near marginality. Larger Kubo numbers near marginality, as shown in figure 3, reinforce this point, which is also differently stressed by recent works in the plasma edge [11, 38]. The fact that QuaLiKiz behaves better near marginality than Gkw is possibly because the QL closure does not include the long-lived zonal flows that quench transport near marginality in GD approaches [17]. In QuaLiKiz, stable modes are neglected, and the turbulent intensity spectrum is fitted [30, 41] onto databases of GD nonlinear computations, similar to those presented here with Gkw. With this procedure, QL models inherit the shortcomings of the primitive GD models onto which they are adjusted. The near marginal transport shortfall in QuaLiKiz indeed largely comes from issues with the QL closure, i.e. the choice of saturation rule and not the QL reduction, per se.
The QuaLiKiz–Jetto framework provides a step towards coupling fluctuations with mean dynamics. This framework emphasises a similar near-marginal flux underprediction, well reproduced by the similar yet fully nonlinear framework of Gene–Tango. This is further indication that the leading-order problem is likely the assumption of a scale separation between ‘equilibrium’ mean scales and fluctuating scales, the latter not being able to feed back onto the former. In the case of QuaLiKiz, this scale separation is inherited from the choice of the saturation rule.

This provides directions for improvement. In physical terms, near-marginal regimes require a description of transport below or at linear stability and of possible coupling to modes presently predicted as stable in QuaLiKiz. Importantly, they also require modelling of the self-advection (spreading) of turbulent domains and the possibility of non-monotonic flux–gradient relations. Several routes can be explored. In the spirit of current frameworks, QL models could be trained on near-marginal FD databases, such as those provided by the likes of GYSELA. This would likely lead to QL closures with regime-dependent turbulent intensity spectra. Alternatively, to present closures, QL models could also be coupled to dynamic equations for the turbulence intensity, e.g. in the form of reaction–diffusion [49] or $k – \epsilon$ equations [50], enriching accessible nonlinear dynamics.

The present work provides a framework of understanding. Ongoing studies are concerned with further characterising the above threshold and near-marginal regimes [51] when kinetic features of electron dynamics are present. This is important to assess the relevance for ITER extrapolations. Electron dynamics are indeed known to locally modify turbulence organisation near low-order rational surfaces [52] yet, interestingly, key features of near-marginal turbulence with Boltzmann electrons (flow patterning, shear effectiveness and staircase organisation)—central here to the near-marginal regime—robustly endure in kinetic electron regimes [39].

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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