Crucial role of zonal flows and electromagnetic effects in ITER turbulence simulations near threshold

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Abstract. A primary component of a validated integrated modeling framework is an accurate transport model describing small-scale, gradient-driven plasma microturbulence and associated cross-field transport. Design and calibration of accurate transport models requires a database of well-converged nonlinear gyrokinetic simulations. Past experience with GYRO simulation of ITER predictive modeling estimates suggested that fusion performance assessments were sometimes pessimistic because turbulent transport was overestimated by the TGLF model. The key feature missing from TGLF was nonlinear zonal-flow generation which can have a significant stabilizing effect near the turbulence threshold. This is in stark contrast to regimes characteristic of modern-day tokamaks for which GYRO and TGLF are typically in close agreement and transport is well-above threshold. In addition, it was also speculated that transverse and compressional electromagnetic effects could play a role in modeling discrepancies. Over time, it became clear that nonlinear zonal-flow stabilization cannot be ignored in modeling reactor plasmas, and so TGLF must be generalized to include zonal-flow stabilization for this regime. In this report we summarize the sequence of steps required to create gyrokinetic simulation datasets suitable for recalibration of TGLF in the near-threshold regime. When this stabilization is added to TGLF, modeled fusion power increased more than 40% in our standard test case.

1. Research motivation and early observations

Development of a validated integrated modeling framework is a fundamental research task within the US fusion energy program. A primary component of this framework is an accurate transport model describing the small-scale, gradient-driven plasma microturbulence and its associated cross-field transport. Predictions of fusion gain in future devices will depend sensitively on the accuracy of the transport model used. However, design and calibration of accurate transport models requires a database of well-converged nonlinear gyrokinetic simulations – a very computationally challenging undertaking. As early as 2008[1], GYRO [1] simulations of ITER operating scenarios were observed to produce levels of nonlinear zonal-flow (ZF) activity large enough to quench turbulence inside $r/a \sim 0.5$. This observation implied that modeling estimates of fusion power in ITER may have been **pessimistic** because turbulent transport was overestimated. The existence of zonal-flow-dominated, low-transport states persisted even as more accurate and comprehensive predictions of ITER profiles were made using the state-of-the-art TGLF transport model [2, 3]. This was in contrast to GYRO-TGLF comparisons for modern-day tokamaks like DIII-D, for which GYRO and TGLF are typically in close agreement [4, 5, 6] and transport is well-above threshold. It was speculated and subsequently verified that ZF generation was an important effect close to threshold and played a key role in reducing the levels of turbulence. In this regime it was also observed that electromagnetic corrections to the transport were non-negligible. Importantly, it became clear that TGLF

[1]J. Candy, *Progress on TGYRO: The Steady-state Gyrokinetic Transport Code*, 21st US Transport Taskforce Workshop, Boulder, CO (March 2008)

must be generalized to include ZF stabilization for more accurate ITER predictive simulations. Exhaustive nonlinear gyrokinetic studies to support TGLF recalibration efforts, which represented an enormous undertaking, were carried out in stages over a period of years. In this report we summarize the key features and more problematic aspects of these studies.

2. Near-threshold regime for ITER simulations

ITER modeling [3] has shown that acceptable energy confinement requires core ion/electron energy fluxes to be on the order of a single gyroBohm; that is, $Q_e/Q_{\rm GB}, Q_i/Q_{\rm GB} \simeq 1$, where $Q_{\rm GB} \doteq n_e T_e c_s \, (\rho_s/a)^2$ is the gyroBohm energy flux, ρ_s is the ion-sound gyroradius, and a is the midplane minor radius of the last closed flux surface. In cases with low levels of equilibrium rotational shear, this level of transport implies a close proximity to the linear instability threshold for the ion-temperature-gradient (ITG) modes. GYRO [1] simulations show that nonlinearly-generated zonal flows are very active under these conditions and lead to *turbulence suppression* (the so-called *Dimits-shift* regime [7]) and bursty (intermittent) transport. Nonlinear gyrokinetic simulations under these conditions are problematic – and more challenging – than cases well above threshold due to the difficulty in obtaining statistically robust estimates of (time-averaged) mean transport levels.

In the baseline case studied in this report, we observe that for steady-state ITER profiles predicted by TGLF, GYRO simulations exhibit weak linear ITG instability. However, the early-time burst of turbulence is subsequently quenched by zonal-flow activity at radii inside about $r/a = 0.6$ (where $r = r_{\rm min}$ is the half-width of the flux surface). An illustration of this turbulence-suppression effect is shown in Fig. 3. Thus, to accurately characterize the transport using in regime, any transport model must include **both** a good approximation to the linear critical gradients, as well as some inclusion of zonal-flow stabilization. In what follows we will specify a hierarchy of new benchmark/calibration cases relevant to the near-threshold regime.

3. Hierarchy of ITER gyrokinetic simulation cases

All profile predictions herein are made using the TGYRO tranport solver [8], based on an ITER hybrid DT scenario with approximately 45 MW of auxiliary power, hollow q-profile, equal D/T fractions, and thermal ^{4}He ash. Impurity ions (Ar, Be, W) and fast-ion populations are also retained in the most complete scenario definition, but we have established that neglect of these species during TGYRO simulation leads to only small errors in profile prediction. For this reason, we consider only three gyrokinetic ions (D, T, ^{4}He) in the subsequent modeling. In TGYRO, alpha heating to electrons and ions, collisional exchange, and electron radiation are computed self-consistently. Neoclassical transport for all species is computed by NEO [9] without approximation. Using 8 TGYRO simulation radii (plus a point on the magnetic axis at which fluxes equal zero exactly), we compute steady-state temperature profiles such that the corresponding gradients serve as nominal ones. The total fusion power for this case, inside $r/a = 0.8$, is about 500 MW. This prediction uses unmodified TGLF as the transport model, with no direct reference to GYRO simulations.

The ITER simulation strategy went through 3 distinct iterations in order to create the most suitable simulation database. The process began by choosing 3 reference radii at which to assess the turbulence levels: $r/a = (0.4, 0.5, 0.6)$. In this section we summarize the nominal local parameters required for nonlinear gyrokinetic transport simulation at these radii. The profiles (and in particular the local gradients) are exactly those computed by TGYRO-TGLF predictive simulation (circa 2014). This *near-marginal regime* is in contrast to the original database of simulations used to calibrate TGLF (see, for example, [10]), which were *well-above* the transport threshold. Thus, the (relatively weak) gradients characteristic of this predicted range will be used to design test cases. First, in Table 1, we summarize the local geometric parameters for our reference reactor scenario. Next, in Table 2, we list local plasma profile parameters. Finally, in Table 3, we give the nominal gradients which can subsequently be adjusted to bring the system closer to, or farther from, threshold. Note that in all cases (2 ion and 3 ion) we use a nearly 50-50 DT mixture. In cases with helium ash impurity, the helium density is taken to be about $n_{\mathrm{He}}/n_e \sim 0.015$.

Table 1. ITER Scenario Local Geometric Parameters

Local parameter	$r/a = 0.4$	$r/a = 0.5$	$r/a = 0.6$
ρ_{tor}	0.3613	0.4531	0.5480
R_0/a	3.2384	3.2232	3.2051
q	1.5688	1.6961	1.8838
s	0.2253	0.4728	0.6833
κ	1.5076	1.5074	1.5194
s_κ	-0.0218	0.0218	0.0689
δ	0.0732	0.0930	0.1176
s_δ	0.0698	0.1098	0.1617
$-\Delta$	0.1385	0.1664	0.1942
$B_{\mathrm{unit}}(T)$	7.6724	7.9257	8.2809

Table 2. ITER Scenario Profile Parameters

Local parameter	$r/a = 0.4$	$r/a = 0.5$	$r/a = 0.6$
T_i/T_e	0.9698	0.9731	0.9719
$\beta_{e,\mathrm{unit}}(\%)$	1.0638	0.8652	0.6871

Table 3. ITER Scenario Nominal Gradients

Local parameter	$r/a = 0.4$	$r/a = 0.5$	$r/a = 0.6$
a/L_n	0.2696	0.2276	0.3429
a/L_{Ti}	1.1301	1.1379	1.1748
a/L_{Te}	1.2262	1.1096	1.1776

Iteration 1: *Nominal gradient simulations, full electromagnetism*

As noted in the previous section, the TGLF recalibration process started with ITER profiles predicted by TGLF. The results confirmed that TGLF **overpredicted** the total energy flux in low-collisionality ITER plasmas. A sample of two cases illustrating this are shown Fig. 1, in which fully-electromagnetic, 3-field ($\delta\phi, \delta A_\parallel, \delta B_\parallel$) simulations with 3 ion species (D,T,He) and kinetic electrons are summarized.

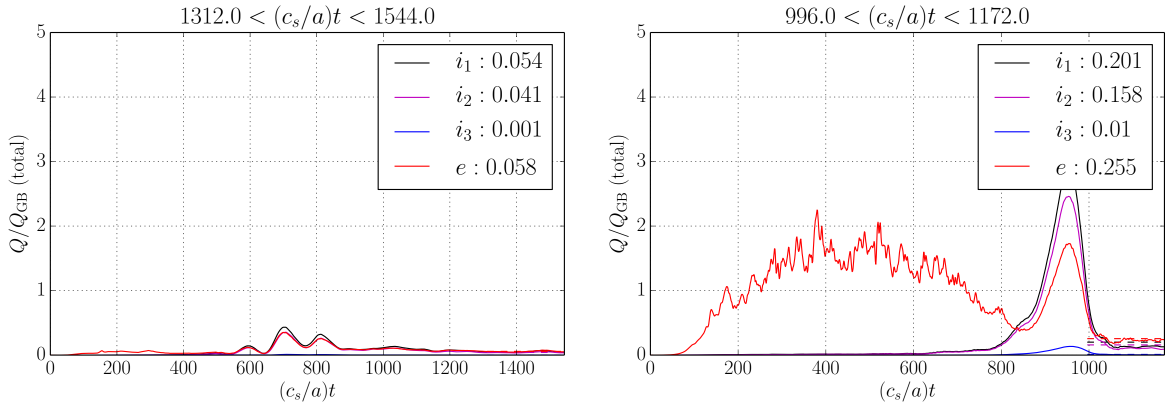

*FIG. 1. Sample 3-field, 3-ion GYRO simulations based on full ITER geometry. Steady-state plasma profiles (and thus gradients) used as input were computed by independent TGYRO-TGLF transport simulations. Left panel shows $r/a = 0.4$ and right panel shows $r/a = 0.5$. This result illustrates the key motivation of the present work: for profiles predicted by (unmodified) TGLF, GYRO shows that turbulence is **completely quenched** in the ITER core by nonlinear zonal-flow generation.*

Iteration 2: *Electrostatic simulations, modified gradients*

The next step was to simplify the cases by switching from 3 ion species (D,T,He) to 2 (D,T), as well as make the fluctuations purely electrostatic. With these simplified assumptions it was more efficient to carry out exhaustive gradient scans. Sample results are shown in Fig. 2. We remark that, in these simulations, the lack of electromagnetic stabilization via neglect of $\delta A_{\parallel}$ *increases* the transport levels somewhat in comparison to the original case of the previous section.

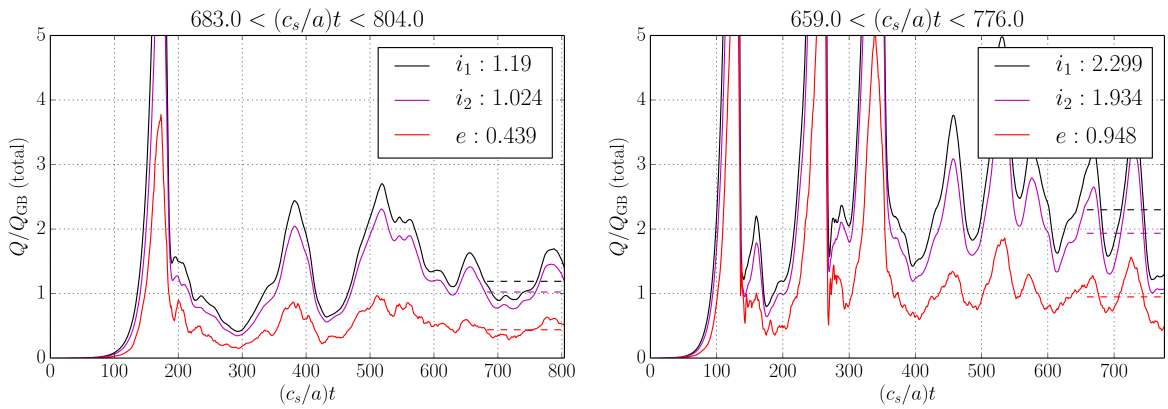

FIG. 2. Sample time-traces of turbulence for electrostatic gradient-scan test case. Left panel shows $r/a = 0.4$ and right panel shows $r/a = 0.5$. These scans were designed to provide a basis for TGLF electrostatic recalibration. Gradients are $a/L_T = 1.25$ for all species – larger than the nominal gradients in Table 3.

Iteration 3: *Simple circular, electrostatic recalibration cases*

An even simpler reactor-relevant test case was constructed that is still fully suitable for transport model calibration in the flow-dominated regime. As before, the simulations used a 2 kinetic ions (D,T) in equal concentrations, kinetic electrons, and only electrostaic fluctuations. However, we further reduced the geometry to a (finite-aspect-ratio) circle and made other geometric simplifications as detailed in Table 4. Simulations were carried out from well into the flow-dominated regime ($a/L_T = 1.2$), as shown in Fig. 3, to the steady-state turbulence regime above threshold ($a/L_T = 1.6$), as shown in Fig. 4.

Table 4. Fixed plasma parameters for simple circular, nonlinear electrostatic simulations

Parameter	r/a	R/a	$(a/c_s)\nu_{ee}$	T_i/T_e	q	s	a/L_n
Value	0.4	3.2	0.015	1.0	1.2	0.6	0.44

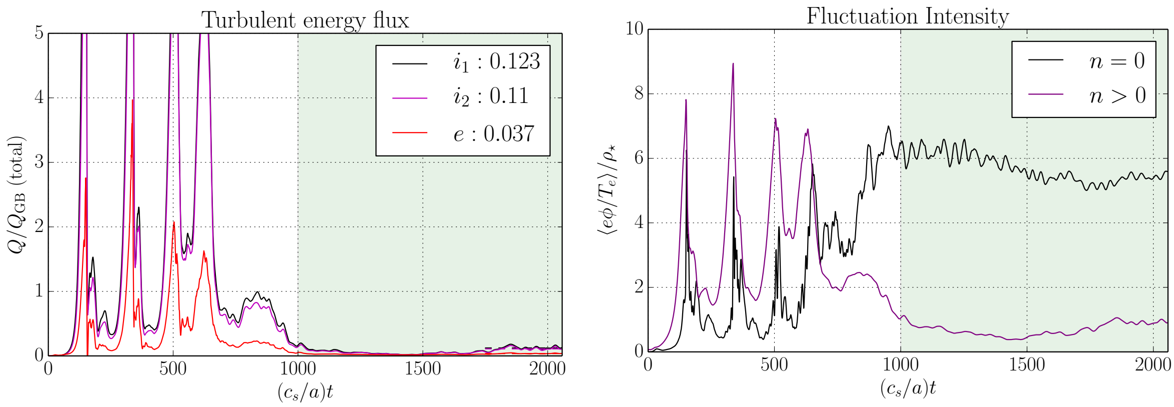

FIG. 3. Simple circular equilibrium, electrostatic nonlinear simulation for $r/a = 0.4$ and $a/L_T = 1.2$ (see Table 4). Left panel shows turbulence time-trace, whereas right panel shows zonal (black) and finite-n (magenta) potentials. Although drift waves are linearly unstable, zonal flows completely quench the turbulence for $(c_s/a)t > 1000$ (green shaded region) after a very long transient phase.

Figure 3 also clearly illustrates a problematic aspect of simulations in the near-threshold regime; namely, the excessive **intermittency** of the GYRO simulations. For these cases we ran the code approximately *four times longer* than standard nonlinear gyrokinetic simulations. Even with the extended simulation times, a steady-state result is not achieved close to threshold. For example, in Fig. 3, there is a finite level of transport for $(c_s/a)t < 1000$, and past this point the system switches to a flow-dominated state with effectively zero transport. This behaviour is rarely encountered when studying existing tokamaks like DIII-D or C-Mod, for which robust steady-states of gyrokinetic turbulence are generally found.

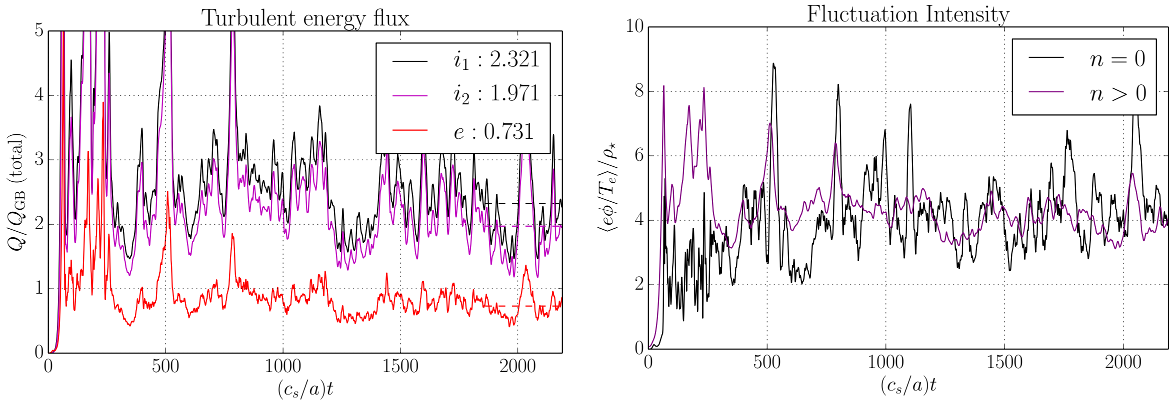

FIG. 4. Simple circular equilibrium, electrostatic nonlinear simulation for $r/a = 0.4$ and $a/L_T = 1.6$. Left panel shows turbulence time-trace, whereas right panel shows zonal (black) versus finite-n (magenta) potentials. In contrast to Fig. 3, this case exhibits well-developed turbulence with relatively good steady-state behaviour.

By studying the interaction of the zonal and drift-wave spectra in numerous cases of this type, a more sophisticated saturation model was developed to replace the original TGLF model. The new model – which we refer to as TGLF-M in this report – gives better agreement with GYRO in the near-threshold regime (compare TGLF-M stars to GYRO squares in Fig. 5). Subsequent predictive ITER simulations with the TGLF-M model showed that the provisional inclusion of ZF stabilization increases the predicted fusion power (versus the original TGLF) by a remarkable 44% – from 470 MW to 676 MW in our test case.

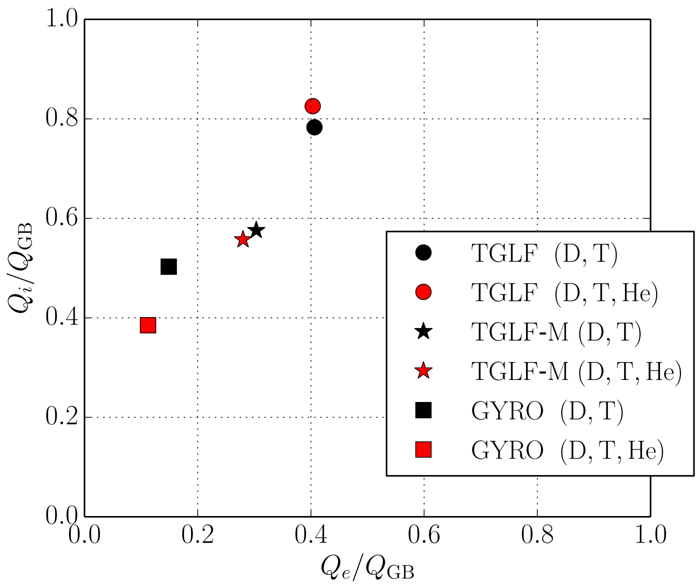

FIG. 5. Comparison of original TGLF (circles), recalibrated TGLF-M (stars) and GYRO fluxes (squares) for new ITER operating point. The new higher-performance operating point was computed by TGYRO using the recalibrated TGLF-M. Simulations include $\delta A_\parallel$ but not $\delta B_\parallel$. Full geometry was used with no approximations. Black symbols indicate 2-ion simulations, red symbols indicate 3-ion simulations. TGLF-M shows a reduction in transport, and thus an improvement in accuracy, in comparison to the uncalibrated TGLF. Q_{GB} is the gyroBohm unit of flux.

4. The effect of magnetic compression

With the improved TGLF model (TGLF-M), we reanalyzed the ITER plasma described in Section 3. The simplifying assumptions were relaxed, so that detailed geometry, and recalculated profiles were considered together with 3 kinetic ion species. In Fig. 6, a surprising result related to electromagnetism is now apparent: the magnetic compression from finite $\delta B_{\parallel}$ contributes an important **destabilizing effect** on the ITG (and a stabilizing effect on the trapped-electron modes). Incorporating magnetic compression is a new challenge for TGLF since $\delta B_{\parallel}$ terms are unchecked and preliminary results do not recover the GYRO trend. In the past, for typical tokamak operating regimes (well above threshold), magnetic compression has been observed to exert only a relativey small effect on drift wave growth rates. However, in the near-threshold regime for ITER parameters, we observe a stronger effect that should not be neglected without further study.

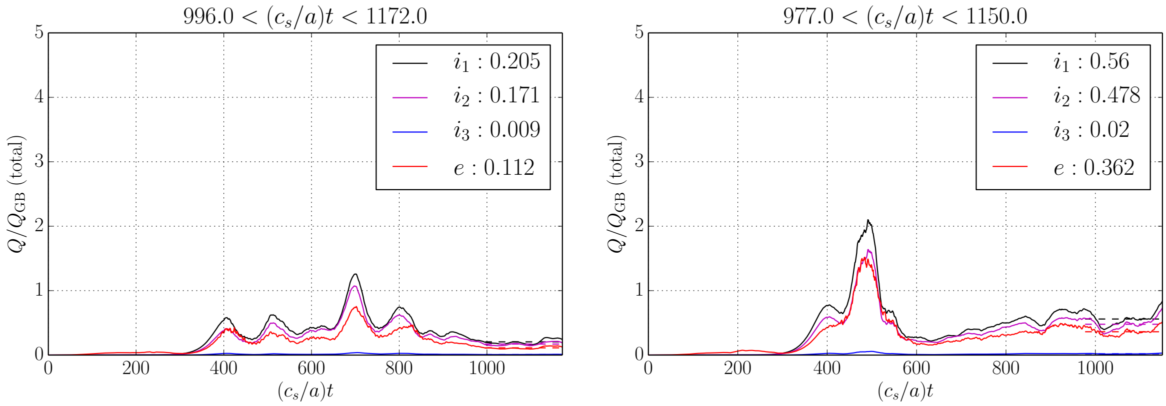

FIG. 6. GYRO simulations for turbulence levels computed using TGYRO with the TGLF-M (recalibrated) transport model. Left panel shows simulation with only transverse magnetic fluctuations ($\delta A_{\parallel}$), and right panel shows full compressional dynamics ($\delta A_{\parallel}, \delta B_{\parallel}$). This result indicates that compressional dynamics (not accurately retained in any transport model) can significantly alter the turbulence level in the near-threshold regime.

5. Tackling electron-scale energy transport

A final issue that warrants significant future research effort is determination of the high-k electron energy flux driven by electron temperature gradient turbulence (ETG). In TGLF, this was initially assumed to be independent of the zonal flow effect, but fluctuation spectra from recent multiscale GYRO simulations by Howard [11] provided a critical new insight. These simulations suggested that ZF advection strongly suppressed electron-scale turbulence, motivating a preliminary new model for ZF saturation of **both** electron and ion-scale turbulence. This preliminary model was recently incorporated into TGLF-M, but ongoing verification of the approach will take time due to the extreme computational expense of multiscale simulation – especially for ITER because of the requirement to treat at least 3 ion species. For this purpose, we have developed a new **multiscale-optimized** GK solver, CGYRO, which is asymptotically more efficient than GYRO for simulations spanning ion and electron space and time scales. With CGYRO we expect to significantly reduce the computational expense of full multiscale simulations for ITER as well as present devices.

6. Summary

In this work, we have shown that for profiles predicted by unmodified TGLF (circa 2012), GYRO simulations demonstrate that turbulence is **completely quenched** in the ITER core by nonlinear zonal-flow generation. When TGLF is modified to account for this zonal-flow stabilization, agreement between TGLF and GYRO is significantly improved, and fusion power predictions for ITER improve by 40% for our test case. We have also demonstrated that for the turbulence regimes characteristic of reactors (sub-gyroBohm ion and electron energy fluxes in the core) nonlinear gyrokinetic simulations are challenging because of the intermittency of fluctuations and related difficultly in achieving steady-state results. Future work will focus on the effects of compressional magnetic perturbations, and more importantly, on multiscale (ion plus electron) turbulence calculations.

7. Acknowledgement

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