Gyrokinetic simulation of a fast L-H like bifurcation dynamics in a realistic diverted tokamak edge geometry

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Different experimental observations in L-H transition

Two different types of experimental observations for the role of the sheared-ExB flow ($V_{\text{ExB}}'$) in edge-turbulence bifurcation:

1. Turbulence generated zonal $V_{\text{ExB}}'$: *Reynolds stress*
   - Yan et al., IAEA16 & PRL14; Schmitz, IAEA16; Tynan, NF13; Istvan PPCF 14, and others

2. Neoclassically generated $V_{\text{ExB}}'$: *X-point orbit-loss* [Chang et al, PoP02]
   - Kobayashi et al., PRL13, and others (X-point orbit-loss)
   - Cavedon, NF17 (Neoclassical)
   - NSTX finds that $P_{L-H}$ is strongly correlated with orbit-loss $V_{\text{ExB}}'$ [Kaye, NF11; Battaglia, NF13]
1. Turbulent zonal $V'_{\text{ExB}}$ & L-H bifurcation in experiment

- $F_{\theta,\text{Reynolds}} = -d<\delta V_r \delta V_\theta>/dr$
- Became basis for the predator-prey model [Kim-Diamond, PRL03, and others]
- When the turbulent Reynolds energy extraction ($\int dt F_{\theta,\text{Reynolds}}$) exceeds the turbulent kinetic energy, turbulence quenching can occur.

**Unanswered questions if Reynolds stress is solely responsible for L-H**
- Right after the turbulence quenching, what is supporting the strong $V'_{\text{ExB}}$?
  - Several experiments report that a strong $\nabla p$ (and its effect on $V'_{\text{ExB}}$) develops only well after a fast bifurcation event [Moyer et al., PoP1995; and others]
- What breaks the symmetry in the $F_{\text{Reynolds}}$, thus the $V'_{\text{ExB}}$, direction?
- Why some machines do not see much Reynolds work?

[Source: Moyer et al., PoP1995]
2. Neoclassically generated $V'_{\text{ExB}}$ & L-H bifurcation in experiment, w/o seeing much Reynolds work

- $V'_{\text{ExB}}$ is driven by $\nabla p$? [Cavedon et al., NF2017, ASDEX-U]
- Orbit-loss-driven $V'_{\text{ExB}}$ [Kobayashi et al., PRL2013, and others]
- NSTX found $P_{L-H}$ is strongly correlated with orbit-loss $V'_{\text{ExB}}$ [Kaye, NF2011; Battaglia, NF2013]

Co-coded flow not seen as bifurcation driver [Kobayashi, NF 2017]

- Could it be possible that the Reynolds stress and orbit loss mechanism work together, with one stronger than the other depending upon the plasma/geometry condition?
- Could the combined Reynolds and X-loss physics provide the missing puzzle pieces in L-H transition physics?
Experimental observations of L-H bifurcation time scale, GAM, and LCO

- When the heating power is close to $P_{LH}$, the bifurcation is observed to be slow with many limit cycle oscillations (I-phase) [Schmitz et al. PRL12 and others]
- When the heating power is $> P_{LH}$, the bifurcation is (forced to be) fast (< 0.1 ms) with an abbreviated I-phase [Yan PRL14, and others]

GAM and Limit cycle oscillation observed as L-mode approaches L-H bifurcation [Conway et al., PRL11]

LCO-type GAMs can be part of the bifurcation physics.
[Conway, PRL 2011]
Why has a gyrokinetic L-H study not been done previously?

Difficulty

- Multiscale in space and time
  - Turbulence
  - Neoclassical with ion orbit loss
  - Neutral particles with ionization and charge exchange
- Magnetic separatrix \((q=\infty)\), which interfaces two different magnetic topologies
- Nonlocal physics
  Radial turbulence correlation width ~ plasma gradient scale length ~ ExB shearing width ~ neutral penetration length
- Large amplitude nonlinear turbulence: \(\delta n/n > 10\%
- Non-Maxwellian plasma
  - Requires fully nonlinear and conserving Collisions

→ Total-f simulation with ~100X more number of marker particles than delta-f simulation in the complex edge geometry: XGC.
→ We thought it would require >100PF computer, non-existent in US yet.
Previously, compute resources discouraged us from studying the L-H transition physics

If we were to establish a global transport-equilibrium in an L-mode plasma, move toward the bifurcation by quasistatically increasing \( P_{\text{heat}} \), go through the bifurcation, and build up pedestal, we would not have enough compute resources to study the transition.

\[ \rightarrow \text{Requires } >10X \text{ faster computer than Titan at ORNL.} \]

**A new strategy** to make the transition physics study possible on Titan:

- Bifurcation may not be a global transport-equilibrium phenomenon
  - But a localized phenomenon at edge
  - May not need to wait until the global non-transport-equilibrium GAMs die out

- Study only the edge bifurcation itself, as soon as the L-mode edge turbulence is established.
  - Force the bifurcation by having \( P_{\text{edge}} >> P_{\text{LH}} \)
  - Experimentally, a forced L-H bifurcation action could be completed in \(<0.1ms \) (Yan-McKee, PRL2014, and others).
  - Take advantage of the fast establishment of edge physics

- Low beta electrostatic simulation
In the core plasma, $f$ evolves slowly

For this argument, let’s use the drift kinetic equation
\[
\frac{\partial f}{\partial t} + (v_{\parallel} + v_d) \cdot \nabla f + \frac{(e/m)E_{\parallel}}{v_{\parallel}} \partial f/\partial w = C(f,f) + \text{Sources/Sinks}
\]
where $w$ is the particle kinetic energy.

In a near-thermal equilibrium, we take the “transport ordering” (= diffusive ordering):
\[
\frac{\partial f}{\partial t} = O(\delta^2), S = O(\delta^2), \text{ with } \delta << 1
\]

- Let $f = f_0 + \delta f$, with $\delta f / f_o = O(\delta), \delta << 1, v_d / v_{\parallel} = O(\delta), E_{\parallel} / m = O(\delta \text{ or } \delta^2)$

$O(\delta^0)$: $v_{\parallel} \cdot \nabla f_0 = C(f_0, f_0) \Rightarrow f_0 = f_M$: H-theorem

$O(\delta^1)$: $\partial \delta f / \partial t + v_{\parallel} \cdot \nabla \delta f + v_d \cdot \nabla f_0 + \frac{(e/m)E_{\parallel}}{v_{\parallel}} \partial f_0 / \partial w = C(\delta f)$

- Perturbative kinetic theories then yield transport coefficients = $O(\delta^2)$
- In this case, fluid transport equations ($f_o \rightarrow n, T$) can be used with the kinetically evaluated or ad hoc closures

$\rightarrow$ GK simulation is cheaper per physics time, but $\delta f$ equilibrates on a slow time scale $O(\delta^1 \omega_{bi}) \sim ms$. And, a meaningful time evolution of $f_0$ in $V_T$ frame can only be obtained in a long “transport-time” scale $O(\delta^2 \omega_{bi})$. $V_T$ evolves on an even slower time scale.
In edge plasma, \( f \) evolves fast

- Ion radial orbit excursion width \( \sim \) pedestal width & scrape-off layer width
- Orbit loss from \( \psi_N < 1 \) and parallel particle loss to divertor

All terms can be large: \( \sim \) either \( O(\omega_{bi}) \) or \( O(\nu_C) \)

- \( \mathbf{v}_\parallel \cdot \nabla f \sim \mathbf{v}_d \cdot \nabla f \sim C(f,f) \sim eE_\parallel \mathbf{v}_\parallel /m \partial f / \partial w \sim O(\omega_{bi}) \sim 0.05 \text{ ms in DIII-D} \)
- \( f \) equilibrates very fast: \( \partial f / \partial t + (\mathbf{v}_\parallel + \mathbf{v}_d) \cdot \nabla f (e/m) + E_\parallel \mathbf{v}_\parallel \partial f / \partial w = C(f,f) + S \)
- If \( S_{\text{neutral}} \) is small, it does not affect the fundamental structure of \( f \).

Fast-evolving nonthermal kinetic system: expensive per physics time \( \rightarrow \) extreme scale computing. However, a short time simulation (~0.1X) can yield meaningful physics.

The edge turbulence around the separatrix saturated before the central core turbulence even started to form
**XGC gyrokinetic codes** (V&V summary at epsi.pppl.gov)

**XGC1: X-point Gyrokinetic Code 1**
- Gyrokinetic ions and electrons
- Lagrangian PIC + Eulerian 5D grid
- Heat and momentum source in core
- Monte Carlo neutrals with wall recycling
- Fully nonlinear Fokker-Planck Coulomb collision operation
- Logical wall-sheath
- Unstructured triangular mesh
- EM with fully implicit drift-kinetic electrons (partially verified).

**XGC1-hybrid: GK ions + fluid electrons**
- Implicit fluid electrons (Hager PoP17)

**XGCa: Axisymmetric gyrokinetic version of XGC1**

**XGC0: Axisymmetric and flux surface averaged drift-kinetic version**

> Full-f + Neutral particles + Unstructured triangular grid
> **Expensive to simulate**
> **Requires extreme scale HPCs**
For the present L-H bifurcation study, we have performed a low-beta electrostatic edge simulation using XGC1.

Plasma input condition
- C-Mod #1140613017 in L-mode, single-null
- $\beta_e \approx 0.01\% < m_e/m_i$ in the bifurcation layer
- $\nabla B$-drift direction has been flipped to be into the divertor

Include the most important multiscale physics
- Neoclassical kinetic physics
- Nonlinear electrostatic turbulence
  - ITG, TEM, Resistive ballooning, Kelvin-Helmholtz, other drift waves
- Neutral particle recycling with CX and ionization
- Realistic diverted geometry

Electromagnetic correction to the present result is left for a future work.
Use a L-mode plasma from C-Mod (beta~0.01%)

Edge temperature increases from heat accumulation

In a developed H-mode pedestal, $dV_E/dr > 0$ at $\Psi_N \sim 0.97$. Any bifurcation mechanism needs to lead to this sign.
Overview of the turbulence behavior at bifurcation

1. $t \approx 0.175-0.21\text{ms}$, suppression of lower frequency, higher amplitude turbulence occurs, and higher frequency, lower amplitude turbulence is generated (shades of green, eddy tearing by $E\times B$ shearing, to be shown).

2. $t > 0.21\text{ms}$, suppression of the lower amplitude turbulence follows.

![Frequency-time spectrum with color scale indicating turbulence amplitude](image-url)
Time-radius behavior of the sheared ExB flow $V_E^\prime$

1. $t=0.12\text{ms}$, $V_E^\prime$ settles down in $\Psi_N \sim 0.97-98$
2. $t<0.17\text{ms}$, positive part of $V_E^\prime$ does not penetrate into the edge layer ($\rho>0$)

Gyrokinetic Poisson Eq. $(\rho_e^2/\lambda_D^2)\epsilon_0 B \ V_E^\prime \simeq e(n_e - n_{i,gc})$

1. $t\sim0.175\text{ms}$, something pushes the $V_E^\prime$ to be $>0$ in the edge layer ($\rho<0$)
2. $t > 0.2\text{ms}$, something then locks the sheared ExB flow into the mean ExB shearing in the bifurcation layer.

Transition layer is at $0.96<\Psi_N<0.98$, agreeing with C-Mod
[Cziegler PPCF2014] and other devices.

[Titan, ALCC 2016]
Detailed local analysis at $\Psi_N=0.975$:

Important physics quantity is the ExB shearing rate, $V_E'$, not $V_E$. The bifurcation criterion is identified to be $V_E' > 300$ kHz (Maximum growth rate of dissipative TEMs [Romanelli PoP 2007]).

$(0.96<\Psi_N<0.98$, per Cziegler PPCF 2014)
Transport fluxes and Reynolds force

• Edge transport fluxes are non-local and follow the GAM behavior, with suppression at the “critical” time.

• The Reynolds force from turbulence $F_{\theta,\text{Reynolds}} = -d<\delta V_r \delta V_\theta>/dr$ fluctuates in both directions, and exhibits shearing

• However, the Reynolds force is a non-player after the bifurcation.

• Questions:
  - What is keeping the turbulence suppressed after the bifurcation?
  - Why is the negative Reynolds force not effective
  - What is pushing $V'_{\text{ExB}}$ further to positive after 0.175 ms?

• It is reasonable to conjecture that there is another force in the positive $V_E'$ direction
The orbit loss physics provides answers to all three questions. [Chang, PoP 2002]
Why does the turbulence get cut-off around 0.18ms? What triggers the bifurcation action?

The normalized, turbulence Reynolds consumption rate 
\[ P = \frac{<\tilde{v}_r \tilde{v}_\theta> V_E}{(\gamma_{\text{eff}} \tilde{v}_\perp^2/2)} \] becomes >1 in the beginning of the bifurcation action (I-phase), but becomes <1 after that \[ \rightarrow \] Zonal flows cannot be responsible for keeping the turbulence suppressed.

[Yan PRL 2014] reported a very similar behavior in the Reynolds consumption rate.

Relevance of the turbulence consumption rate? Eddie-tearing by ExB shearing could also be responsible for this cut-off.
Summary and Discussions

• The total-f XGC family codes have been making important scientific discoveries on leadership class computers, which could not have been possible otherwise.

• A forced, fast L-H like bifurcation dynamics has been revealed, with transport suppression in both the heat and particle channels.

• The turbulent Reynolds stress and the neoclassical X-loss physics work together in achieving the L-H bifurcation.
  - When combined together, the puzzle pieces appear to come together.
  - How will the geometry and plasma condition change their combination? → Neoclassical NSTX could be a good test bed.
  - How will this affect $P_{L-H}$ in ITER where the $E_{r,NEO}$ could be relatively weak?

• Isotope effects may be studied in the near future.

• EM correction to the present electrostatic result will be studied in the future.

• We will study the I-mode bifurcation in the near future.