Latest developments in BOUT++ boundary plasma turbulent transport simulations

2018 BOUT++ workshop

14-17 August 2018, Livermore, CA, USA

Xueqiao Xu

In collaboration with BOUT++ team

LLNL-PRES-756204

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

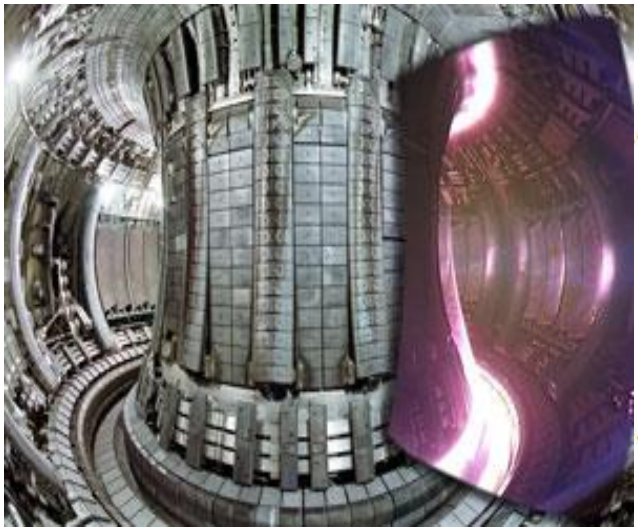
Tokamak edge region encompasses boundary layer between hot core plasma and material walls

- Complex geometry
- Rich physics (plasma, neutral/impurity, material)

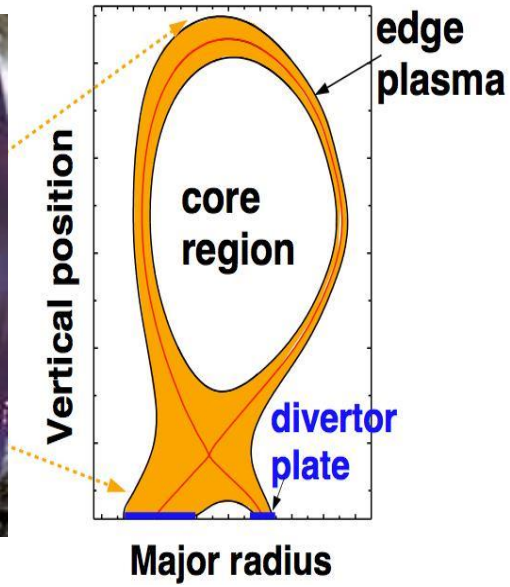
- Sets key engineering constraints for fusion reactor
- Sets global energy confinement

Tokamak interior

Magnetic fusion device



Edge-plasma region



BOUT (BOUndary Turbulence) was originally developed at LLNL in late 1990s for modeling tokamak edge turbulence

BOUT++ is a successor to BOUT, developed in collaboration with Univ. York*

Original BOUT, tokamak applications on boundary turbulence and ELMs with encouraging results

BOUT++

Boundary Plasma Turbulence Code

BOUT-06: code refactoring using differential operator approach, high order FD, verification

4 SciDac centers

- ✓**Tokamak Disruption Simulations**
- ✓**RF-Plasma Interactions**
- ✓**Plasma Surface Interactions**
- ✓**Whole Device Modeling**
- ✓**ITER & CFETR**

BOUT++: OOP, 2D parallelization, applications to tokamak ELMs, blobs/filaments & turbulence

2000 2005 2018

- *Xu and Cohen, Contrib. Plasma Phys. 38, 158 (1998)*
- *Xu, Cohen, Rognlien, Myra, Phys. Plasmas, 7, 1951 (2000)*
- *Xu, Umansky, Dudson & Snyder, CiCP, V. 4, 949-979 (2008).*
- Umansky, Xu, Dudson, et al., , Comp. Phys. Comm. V. *180 , 887-903 (2008).*
- Dudson, Umansky, Xu et al., Comp. Phys. Comm. V.180 (2009) 1467.
- Xu, Dudson, Snyder et al., PRL 105, 175005 (2010).

https://bout.llnl.gov

http://boutproject.github.io

BOUT and BOUT++ have been products of broad international collaborations

IFS Theory Group Institute for Fusion Studies

DEL TECH

THE UNIVERSITY OF CALIFORNIA UCLA

UCSD

GENERAL ATOMICS

Argonne NATIONAL LABORATORY ILLINOIS INSTITUTE OF TECHNOLOGY

DCU

CCFE CULHAM CENTRE FOR FUSION ENERGY

UNIVERSITY of York

BERKELEY LAB Lawrence Berkeley National Laboratory

MIT PSFC

QST

TECH-X SIMULATIONS EMPOWERING YOUR INNOVATIONS

Lodestar Research Corporation

Lawrence Livermore National Laboratory

1920 HIT

HUAZHONG UNIVERSITY OF SCIENCE & TECHNOLOGY

POSTECH 포항공과대학교

ULSAN NATIONAL INSTITUTE OF SCIENCE AND TECHNOLOGY UNIST

XIHUA UNIVERSITY 1960

SICHUAN UNIVERSITY 1896

University of Science and Technology of China 1958

西安交通大學 XI'AN JIAOTONG UNIVERSITY

1896

NFRI 국가핵융합연구소 National Fusion Research Institute

SOONGSIL UNIVERSITY 1897

SWIP

DALIAN UNIVERSITY OF TECHNOLOGY 1949

THE UNIVERSITY of WISCONSIN MADISON

ifts 浙江大學聚變理論與模擬中心 Institute for Fusion Theory and Simulation, Zhejiang University

Southwestern Institute of Physics

Institute of plasma Physics Chinese Academy of Sciences

PEKING UNIVERSITY 1898 北大聚变模拟中心 Fusion Simulation Center, Peking University

32 Institutions Around the Globe

National Labs/Institutes: 8 University: 21 Industrial: 3

- **USA 10**
  LLNL, GA, UCSD, MIT, UW Madison, UCLA, Tech-X, Lodestar, LBNL, ANL

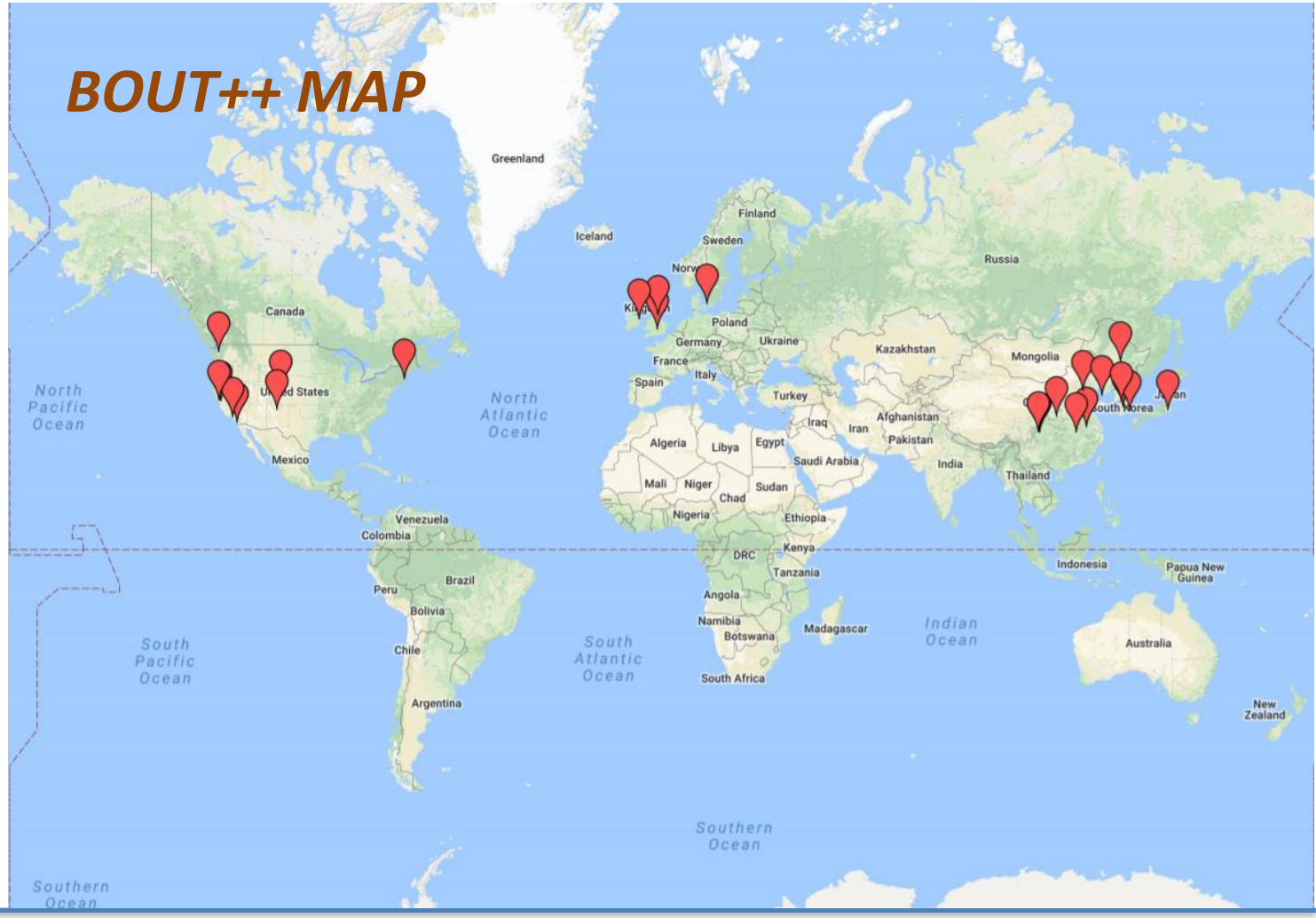
- **Europe 4**
  U York, CCFE, DTU, DCU

- **Asian 18**

  - **China 13**
    ASIPP, Peking U, DLUT, USTC, SWIP, Zhejiang U. HUST, SCU, SWJTU, XJTU, XHU, HIT

  - **Japan 1**
    QST-Rakkasho

  - **Korea 4**
    NFRI, POSTECH, UNIST, Soongsil University

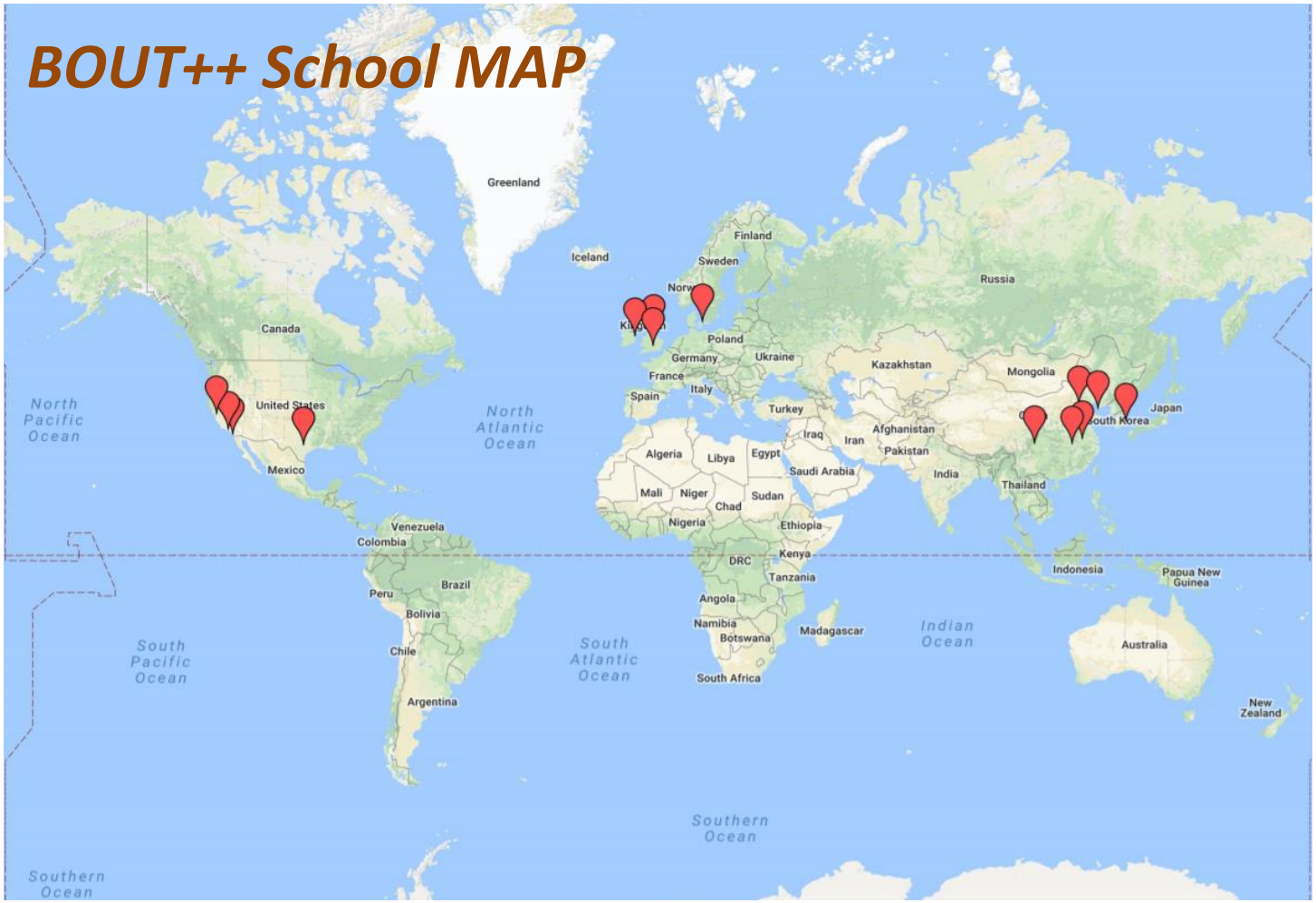


Global PhD training and development program

School (Graduated, Current)

Graduated PhDs: 21 **Current PhD Candidates: 24**

- **USA (3,0)**
  - UCSD (1,0)
  - UCLA (1,0)
  - UT-Austin (1,0)
- **Europe (7,8)**
  - U York (3,2)
  - U York/CCFE (3,4)
  - DTU (1,0)
  - DCU (0,2)
- **China (10,14)**
  - PKU/LLNL (4,4)
  - ASIPP/LLNL (1,1)
  - USTC/LLNL (1,0)
  - DLUT/LLNL (0,3)
  - USTC (0,1)
  - SCU (4,2)
  - DLUT (0,2)
  - HUST (0,1)
- **Korea (1,2)**
  - POSTECH (1,0)
  - SSU (0,2)



BOUT & BOUT++ Work Produced Multiple Publications since 2000

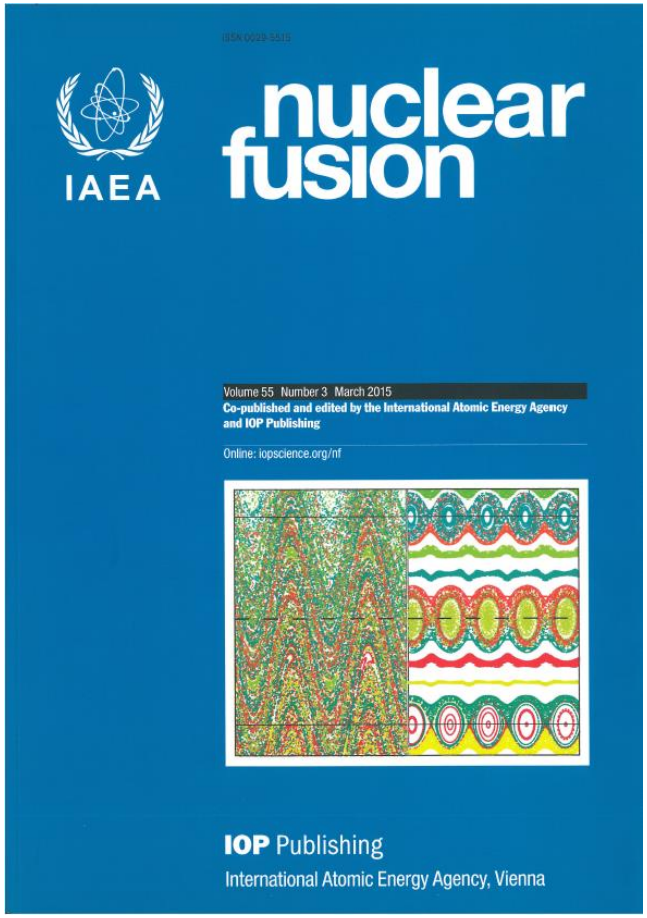
- **Journal Publications, 41+101**
  - ✓ **PRL**
  - ✓ **Nuclear Fusion**
  - ✓ **JCP**
  - ✓ **CPC**
  - ✓ **PoP**
  - ✓ **PPCF**
  - ✓ **JNM**
  - ✓ **Phys. Lett. A**

  ….

- **1 paper selected as a cover paper**
  - ✓ **Nucl. Fusion : March, 2015**

    T Rhee et al, NF 55 032004 (2015)

- **3 paper selected as an editor's pick in Phys. Plasmas**
  - ✓ **T Tran et al,** PoP 24, 102318 (2017)
  - ✓ **Z. X. Liu, et al.,** POP 21, 090705 (2014)
  - ✓ **B. Friedman,** PoP 2013



https://bout.llnl.gov/publications http://boutproject.github.io/publications/

BOUT & BOUT++ Work Produced Multiple Major International Conference Invited/Oral Presentations since 2000

Major International Conferences: 31

- IAEA-FEC: 7=3+4
- PSI 2
- APS-DPP: 14
- EPS 2
- AAPPS-DPP 6

100s talks at various topical and regional conferences

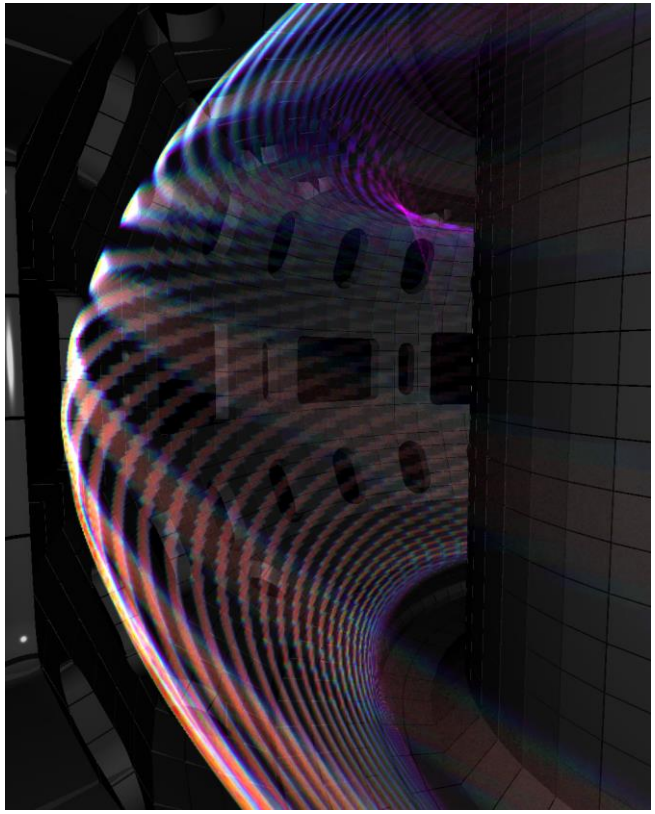
- TTF
  - US
  - EU-US
  - APTWG
- Sherwood
- EFPW
- Varenna-Lausanne workshop
- H-mode workshop
- IAEA technical meeting

….

Oral talks presented at IAEA FEC

1) **X. Q. Xu**, et al., **Turbulence Simulations of X Point Physics on the L-H Transitions,**TH4/4, 18th IAEA FEC, 4-10 October, 2000, Sorrento, Italy
2) **X. Q. Xu**, R.H. Cohen, W.M. Nevins, T.D. Rognlien, et al., **Density effects on tokamak,**, TH/1-5, 20th IAEA Fusion Energy Conference 2004, 1st-6th November 2004, Villamoura, Portugal
3) **P.B. Snyder**, et al., **Stability and Dynamics of the Edge Pedestal in the Low Collisionality Regime: Physics Mechanisms for Steady-State ELM-Free Operation, TH/4-1Ra,** 21st IAEA Conference, Chengdu, 16–21 October 2006
4) **T.Y. Xia**, Five-field Peeling-Ballooning Modes Simulation with BOUT++, TH/5-2Ra,
   X.Q. Xu, ,Theory and Gyro-fluid Simulations of Edge-Localized-Modes, TH/5-2Rb, 24th IAEA Fusion Energy Conference, October 8-13, 2012, San Diego, USA
5) **X.Q.Xu**, et al., **Toward An Emerging Understanding of ELM Crashes and Energy Loss Scaling, TH/3-1Ra,**
   G.Y. Zheng, Divertor Design and Analysis of HL-2M, TH/3-1Rb, 25th IAEA Fusion Energy Conference, October 13-18, 2014, St. Petersburg, Russian Federation
6) **Hogun Jhang**, et al., **Excitation of zonal flows and their impact on dynamics of edge pedestal collapse,** TH/8-3, 26th IAEA Fusion Energy Conference, October 17-22, 2016, Kyoto, Japan
7) **F. Militello**, et al., **Predicting Scrape-Off Layer profiles and filamentary transport for reactor relevant devices**, 27th IAEA Fusion Energy Conference, 22-27 October, 2018, Gandhinagar (Ahmedabad) Gujarat, INDIA.

Principal Results since 2015 BOUT++ workshop



- **Formulation / Theory**
  - Landau Fluid Closures
  - Zonal Flows
- **Code Development**
  - SD1D
  - 2D transport
  - Hermes
  - STORM
  - BOUT++ in OMFIT
  - Pellet injection
  - RF-Plasma Interactions
  - RMP
  - Impurity and Dust Transport
- **Physics Highlights**
  - Divertor heat flux width
  - SOL filamentary dynamics
  - Pedestal instabilities and turbulence

Extended Hammett-Perkins static Landau-Fluid closure to arbitrary frequency and tested in BOUT++

The harmonic average closure is

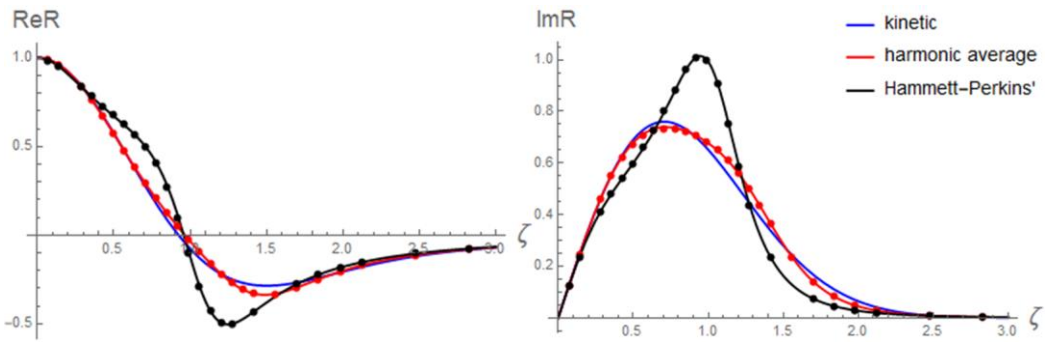
$$\tilde{q} = -\frac{\sqrt{2}n_0 v_t}{\frac{\sqrt{\pi}}{2} - i\frac{2\kappa}{3}\zeta} i\hat{k}\tilde{T}, \qquad \zeta = \frac{\omega}{\sqrt{2}|k|v_t}$$

$$\kappa = \begin{cases} 0 & \zeta \to 0 \quad Hammett - Perkins' 3\ moment \\ 0.53 & \zeta \ll 1 \quad Hammett - Perkins' 4\ moment \\ 1 & \zeta \to \infty \quad Chang - Callen\ limit \end{cases}$$

The closure can be solved using fast non-Fourier method

$$\frac{\partial}{\partial t}\tilde{q} = \frac{3\sqrt{2\pi}v_t}{4\kappa}\frac{\partial}{\partial z}\tilde{r} - 3n_0 v_t^2 \frac{\partial}{\kappa \partial z}\tilde{T}$$

$\tilde{r} = \frac{ik}{|k|}\tilde{q}$ can be calculated by SMHS method



The points are from the simulation result, red is for $\kappa = 0.5$

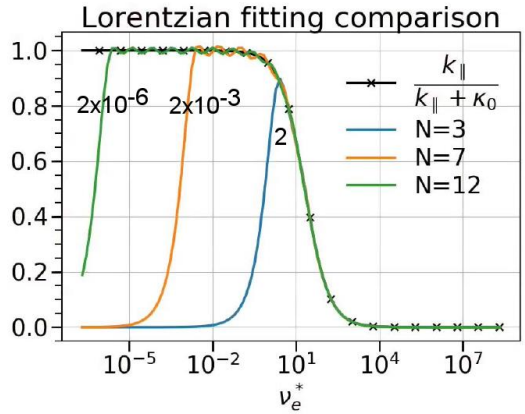
Wang, Xu, et al, in preparation for POP 2018 & poster session I

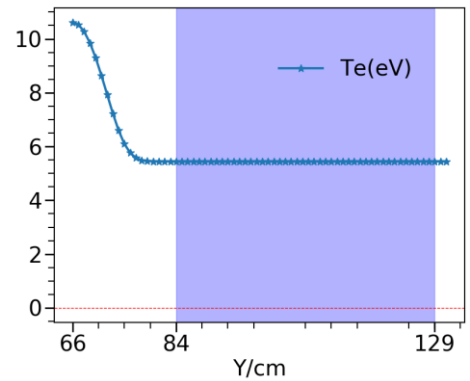
Extended fast non-Fourier method (SMHS) of Landau-fluid closure to weakly collisional regime implemented sheath boundary conditions

$$q_{\|j} = -\kappa_{\|j}\nabla_{\|}T_j$$

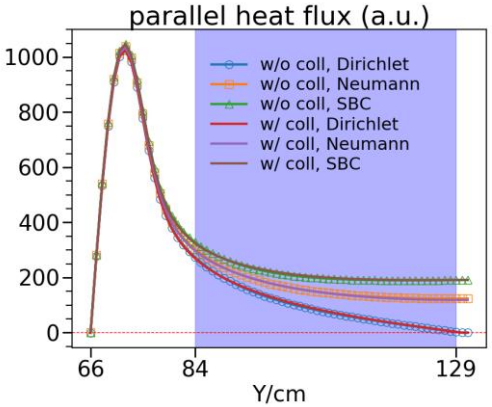
$$\kappa_{\|i}^{\mathrm{SH}} = 3.9 n_i v_{th,i}^2/\nu_i, \quad \kappa_{\|e}^{\mathrm{SH}} = 3.2 n_e v_{th,e}^2/\nu_e$$

Chen, Xu, et al, CPC 2018





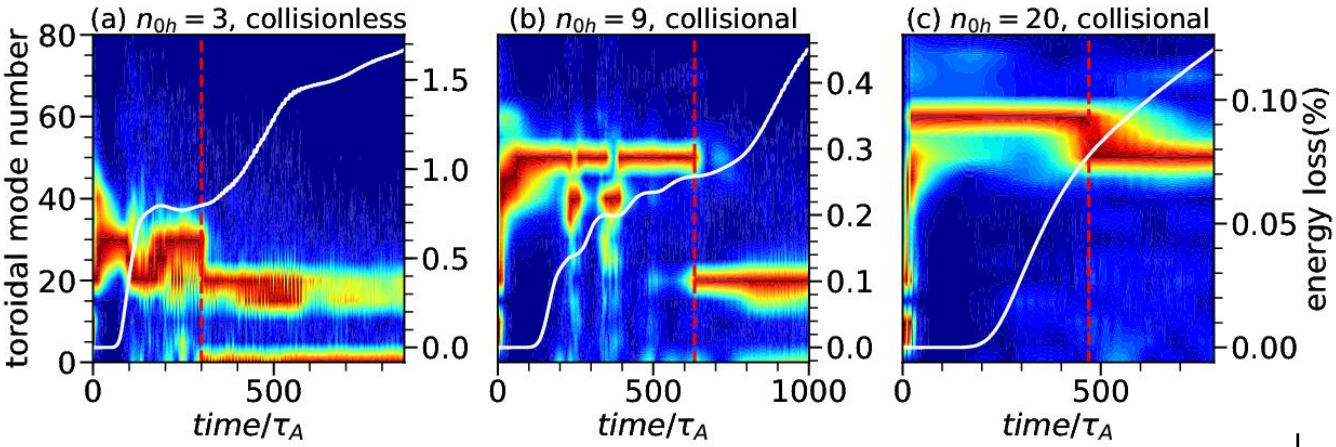
$$q_{\|j,k} = \begin{cases} -A\dfrac{ik_\|\tilde{T}_{j,k}}{|k_\||} \simeq -A\displaystyle\sum_{n=0}^{N-1}\frac{k_0\alpha^n\beta}{k_\|^2+(k_0\alpha^n)^2}ik_\|\tilde{T}_{j,k} = \sum_{n=0}^{N-1} q_{j,k}^n, & \textit{collisionless} \\ -A\dfrac{ik_\|\tilde{T}_{j,k}}{|k_\||+\zeta_0} \simeq -A\displaystyle\sum_{n=0}^{N-1}\frac{\alpha_n/\zeta_0}{(k_\|/\zeta_0)^2+\beta_n^2}ik_\|\tilde{T}_{j,k} = \sum_{n=0}^{N-1} q_{j,k}^n, & \textit{collisional} \end{cases}$$



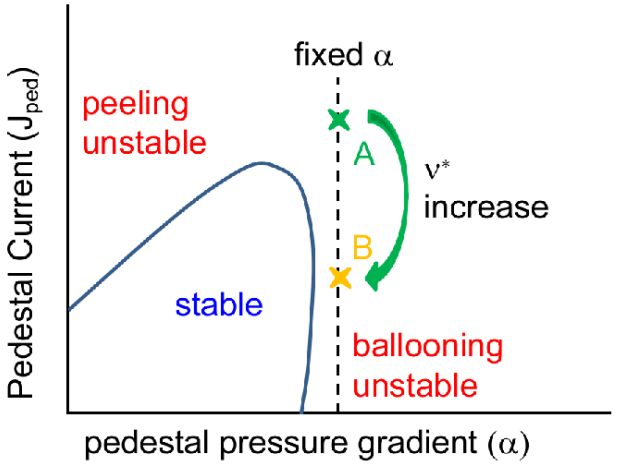
- **Collsionless LF(relative errors 1:16%)**
- **Collisional LF: extended to weakly collisional regime $\nu_e^* \gtrsim 0{:}01$（N=7, ITER)**

- **Collisional limit，collisional LF yields heat fluxes consistent with Spitzer-Härm's results**
- **Weakly collisional limit，strong non-local heat fluxes and sensitive to boundary conditions**

Nonlinear simulations show that increasing bootstrap Current leads to low-n modes to become dominant modes and enhances the energy loss



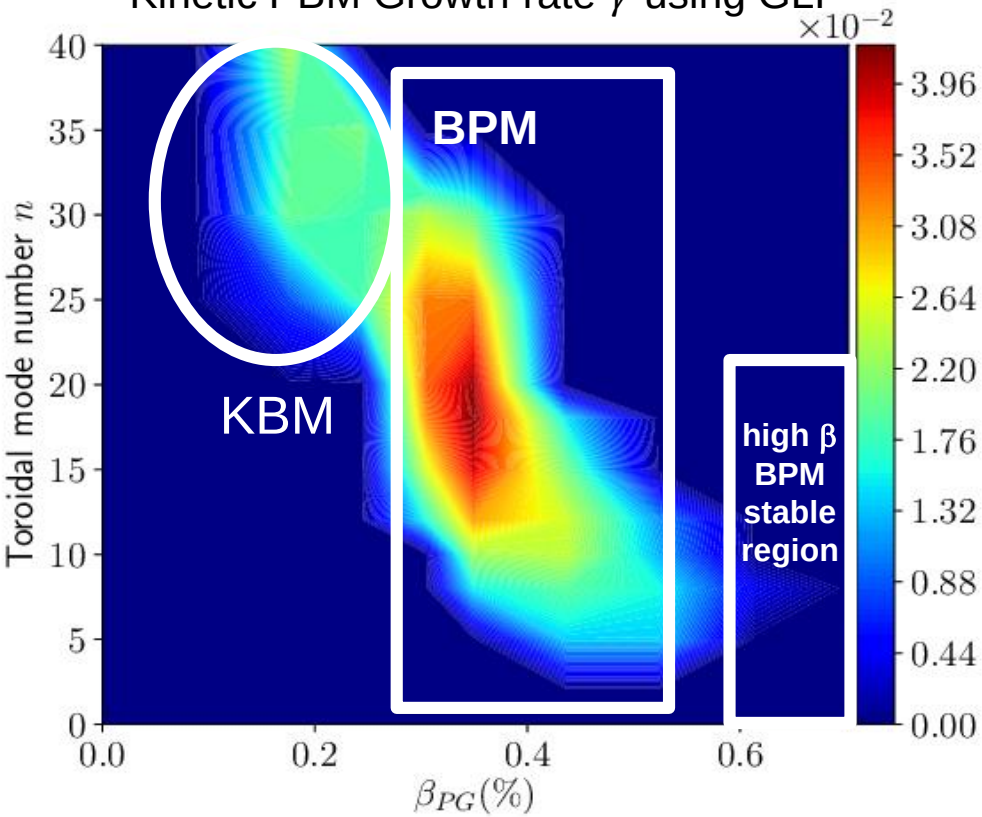
Chen, Xu, et al., PoP 2018



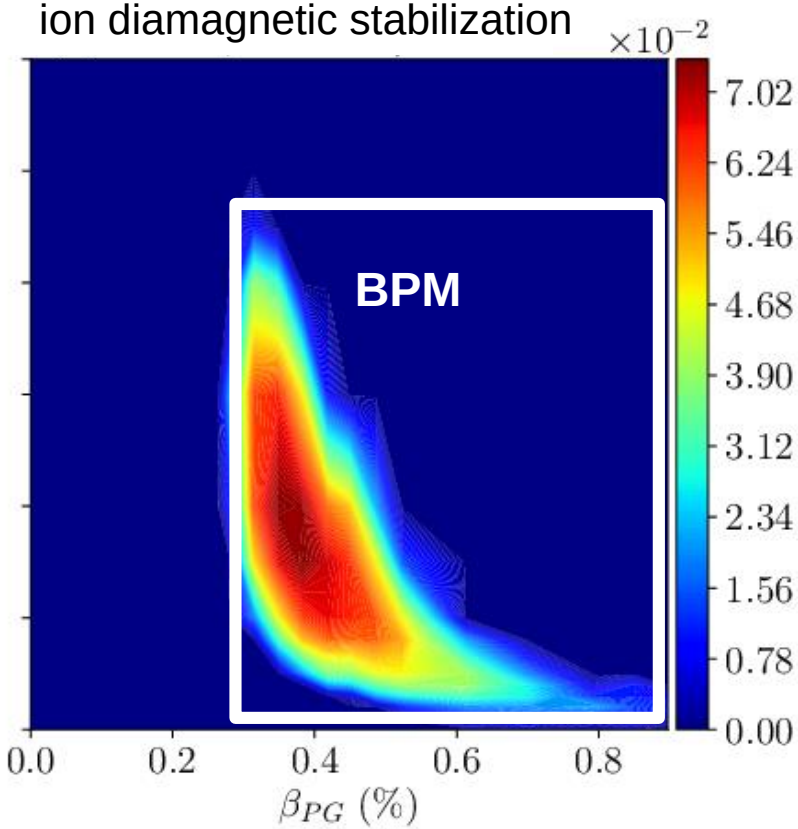
- As density decreases, dominant modes shift to low-n
- Bootstrap current destabilizes the low-n peeling modes stabilizing high-n ballooning modes
- Bootstrap current enhances particle and energy transport and enlarges the radial perturbation domain

Kinetic effects reduce the unstable region of P-B instabilities in β and toroidal mode number n in GLF model

Kinetic PBM Growth rate γ using GLF



PBM using 3-field model with ion diamagnetic stabilization



Sun, Xu, et al., PoP 2018 & poster session II

Kinetic effects using GLF model lead to:
(1) low β KBM unstable; consistent with EPED model; (2) high β BPM stable region

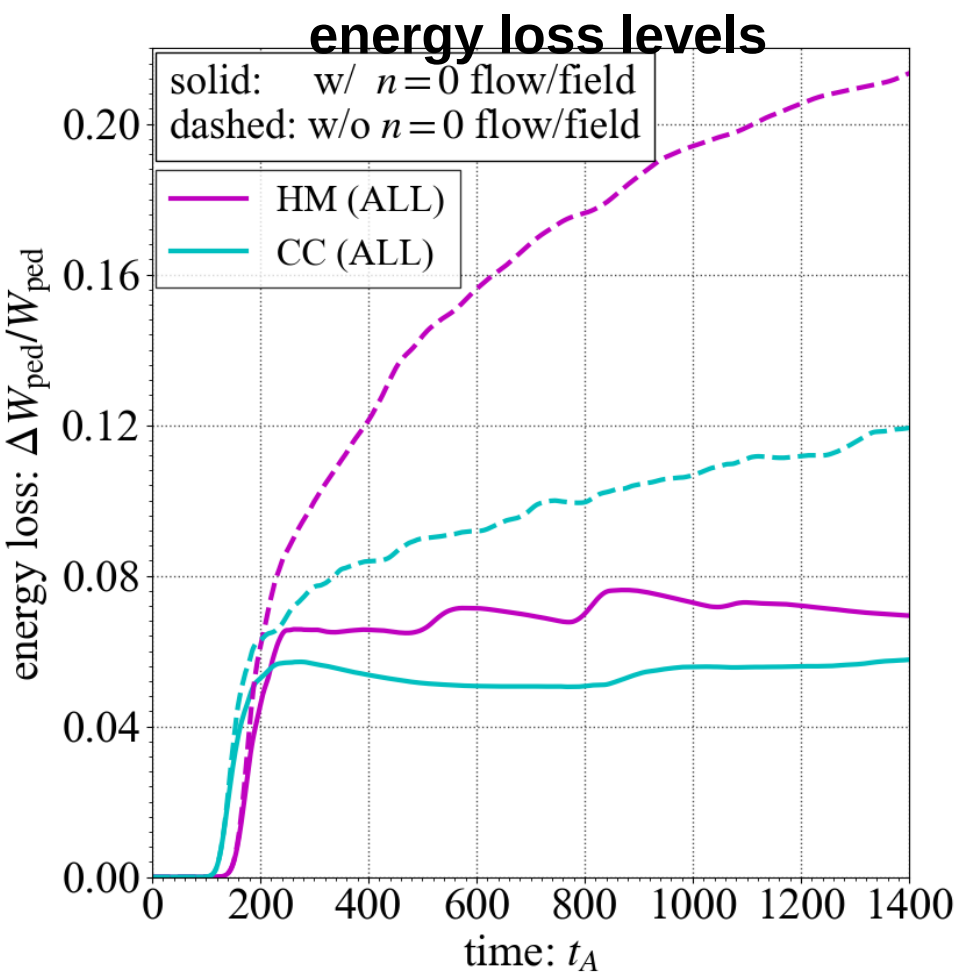
Impact of zonal flow & zonal field on Energy Loss

ELMs with *n*=0 flow/field are simulated by BOUT++ at the first time with Hazeltine-Meiss & Chang-Callen 4-field P-B models

- ***n*=0 flow/field have large impact on ELMs in both models**
- **Energy losses w/ *n*=0 flow/field show considerable difference**

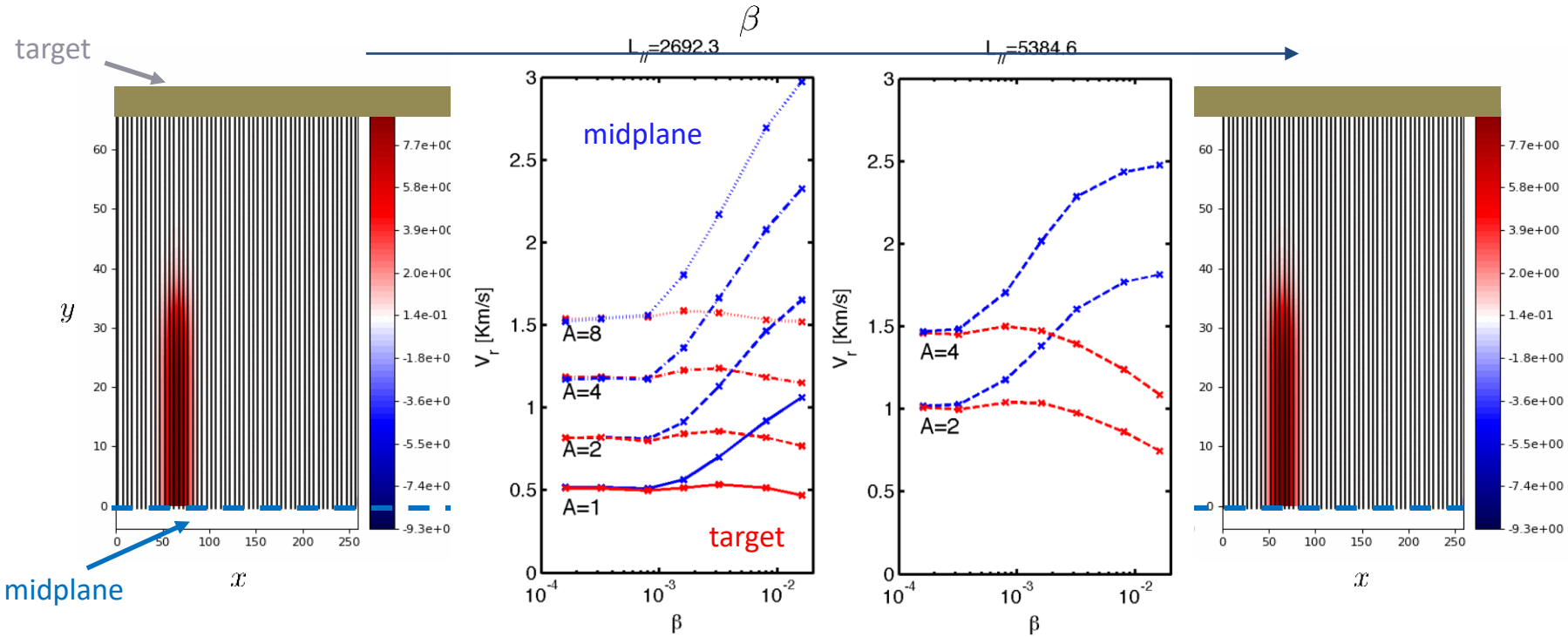
Haruki SETO, talk Tuesday afternoon

Note: energy loss is defined by released energy from ψ=0.86



Electromagnetic effects on filamentary dynamics: STORM

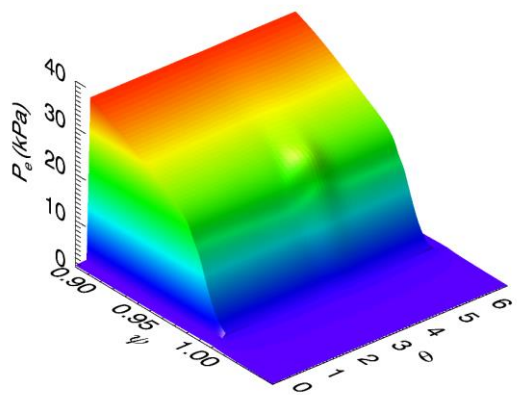
- Do filaments affect field lines?
- Do filaments behave differently when including electromagnetic effects?

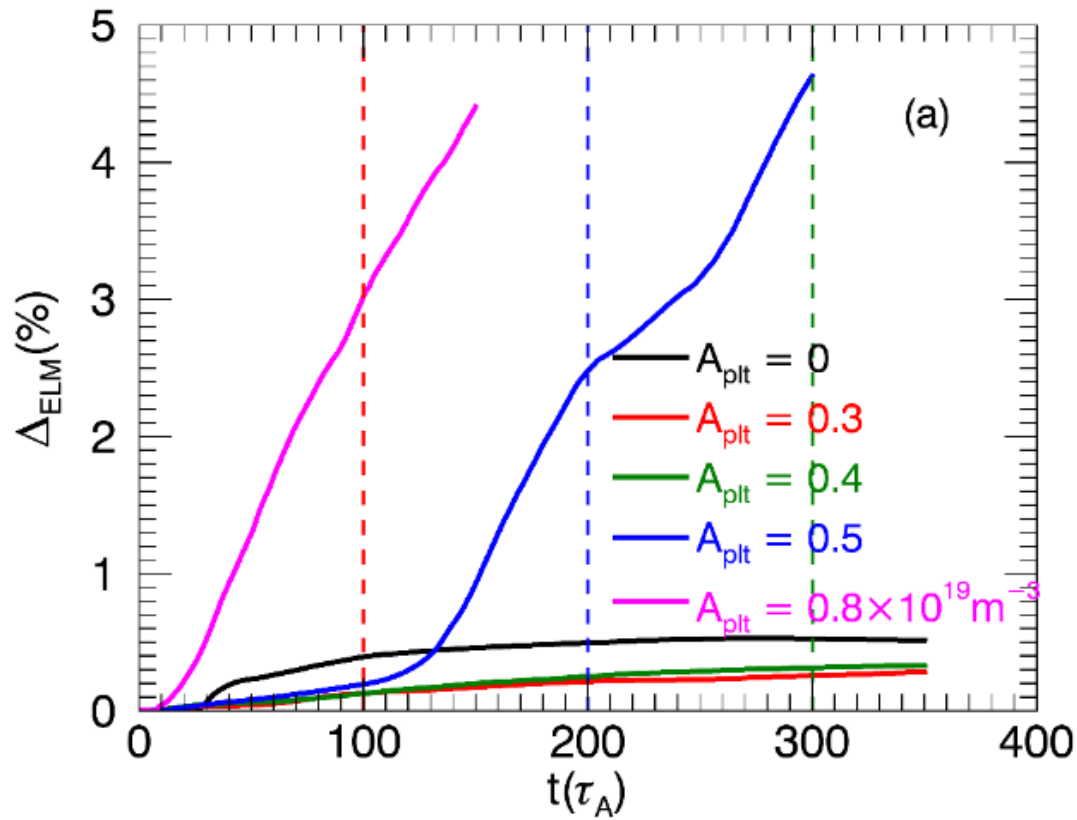


[Hoare *et al.*, in preparation]

Lithium pellet transport study & ELM triggering

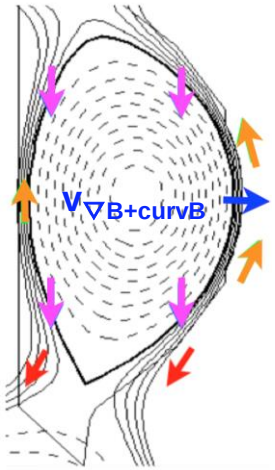
- **ELM triggering study using turbulence code**
  - **The ELMs are triggered when pellet size exceeds a threshold value**
  - **Larger ELMs are triggered when the pellet ablated at the separatrix**
- **Lithium pellet transport study**
  - ✓ **Ablation:**
    Neutral gas shielding mode (NGS)
  - ✓ **Transport:**
    Reduced Braginskii equations for plasmas: e^-, D_i, L_i^{+1}, L_i^{+2}, L_i^{+3}





Wang, Xu et al., submitted to NF 2018 & poster session I

Both EM fluctuation & drifts provide anomalous radial transport, setting divertor heat flux width



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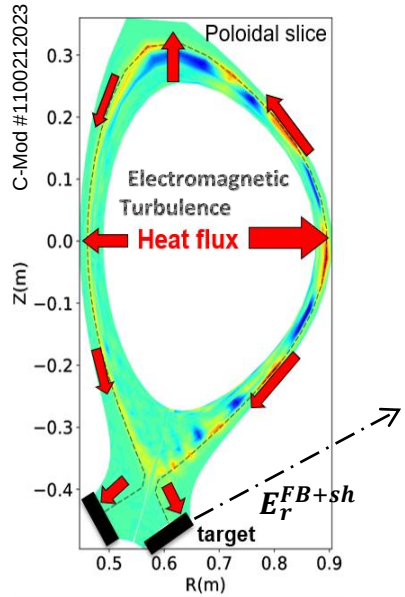
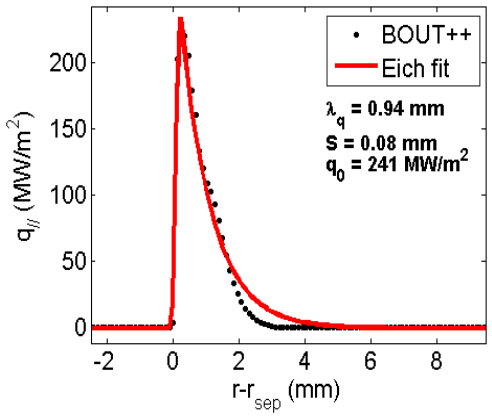




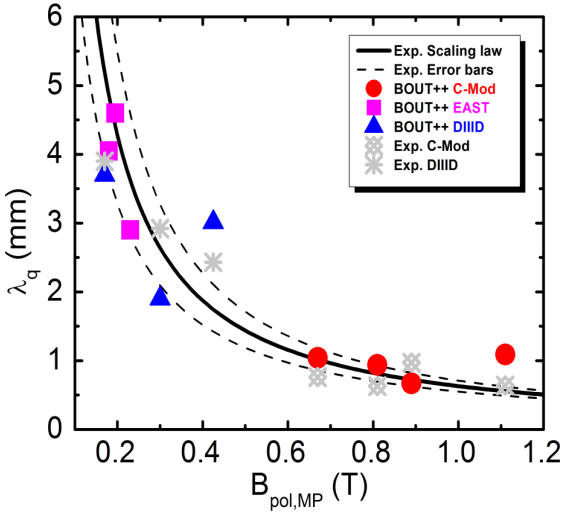
Setting density channel width
$\lambda_n \sim v_{\nabla B+curvB}(L_{||}/c_s) \sim q\rho_s$

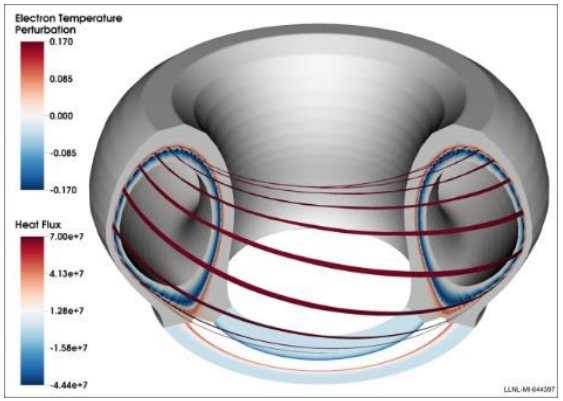
[1] B. Chen, X. Q. Xu, et al, Phys. Plasmas **25**, 055905 (2018).
[2] R. J. Goldston, Nucl. Fusion 52, 013009 (2012);
[3] T. Eich, et al, 2013 Nucl. Fusion 53 093031.

- **Upstream:** **Both EM fluctuations & drifts provide anomalous radial transport**
- **SOL:** **Parallel transport connect SOL to divertor**
- **Divertor footprint:** **Radial profile of divertor heat flux mapped to the outer midplane, showing a good agreement with Eich-fitting formula**

Principal Results

- **BOUT++ turbulence code is used to simulate the electron heat flux width λ_q, which is consistent with experimental Eich scaling**
  - ✓ **The large SOL turbulence originates from the peak gradient region inside the pedestal and not from local instabilities in the SOL**
  - ✓ **Turbulence simulations compared well with data from C-Mod**
- **Transport simulations show that**
  - ✓ **Drifts and turbulent transport are locked in a tight competition for C-Mod**
  - ✓ **ITER & CFETR will possibly be in a turbulence dominant regime**





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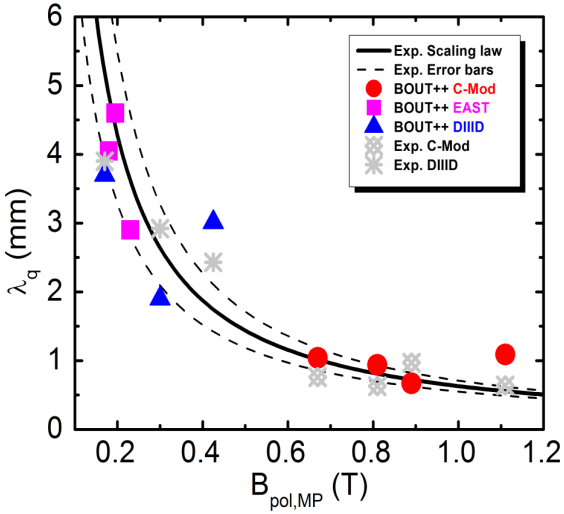

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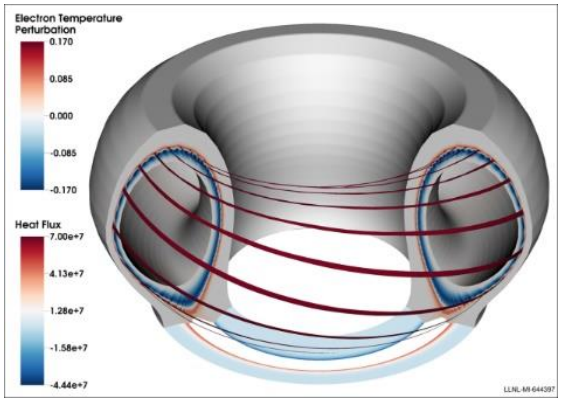
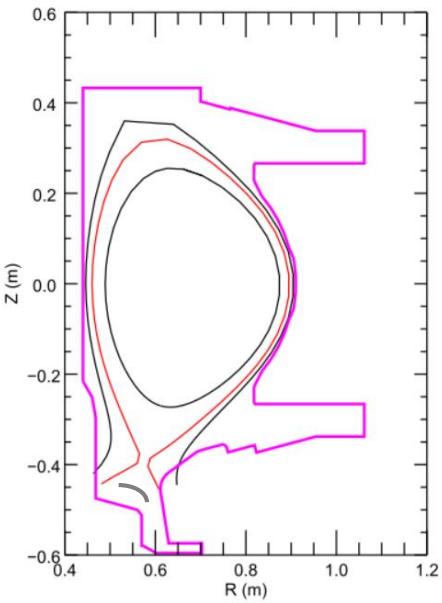


BOUT++ turbulence code is used to simulate the divertor electron heat flux width

- **BOUT++ 3D 6-field 2-fluid evolves**
  - ✓ **density n_i,**
  - ✓ **ion temperature T_i**
  - ✓ **electron temperature T_e**
  - ✓ **parallel velocity $v_{||i}$**
  - ✓ **vorticity ϖ**
  - ✓ **perturbed magnetic vector potential $A_{||}$ for turbulence**

- **To simulate tokamak divertor heat flux width**
  - ✓ **Special source inside the separatrix to maintain the experimentally measured plasma profiles inside the separatrix and let the SOL plasma profiles evolving**
  - ✓ **Flux-limited parallel thermal transport**
  - ✓ **Sheath boundary conditions**



[1] X.Q.Xu et al., PoP **7**, 1951 (2000)
[2] X. Q. Xu et al., Commun. Comput. Phys. 4, 949 (2008)
[3] T. Y. Xia et al., 2013 Nucl. Fusion 53 073009
[4] T. Y. Xia et al., Nucl. Fusion 55, 113030 (2015)

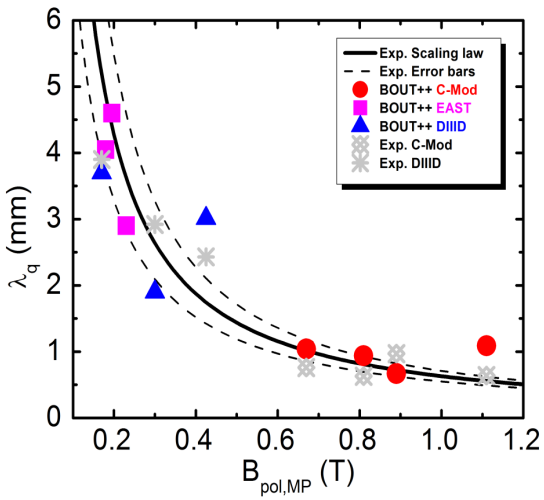
Setup of BOUT++ simulations for the divertor heat load

The inputs to BOUT++ simulations

- **The magnetic geometry**
- **Plasma profiles of each species up to separatrix**
- **This information is taken from the**
  - **C-MOD, DIII-D, EAST experiments;**
  - **ITER and CFETR Scenario studies;**
- **Computation region across the magnetic separatrix**

The outputs from the BOUT++ simulation

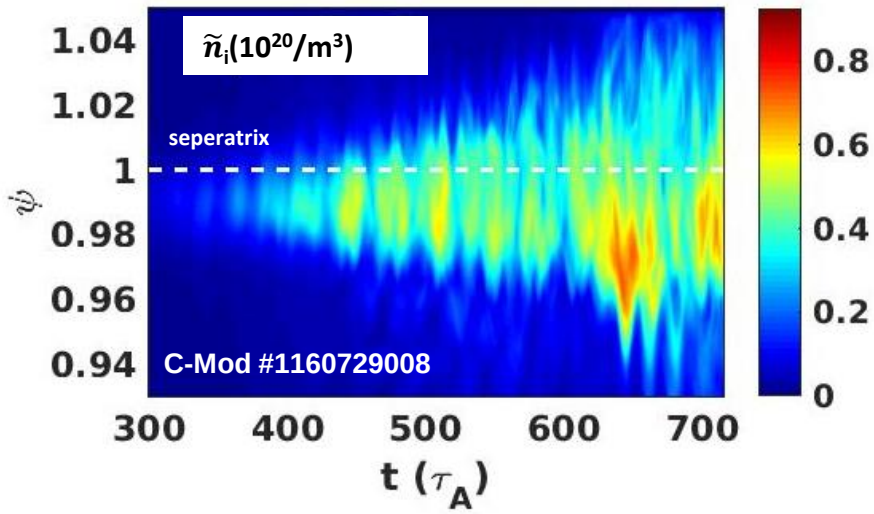
- **Turbulence fluctuation across the separatrix**
- **Power across the separatrix**
- **Divertor heat flux amplitude and width**

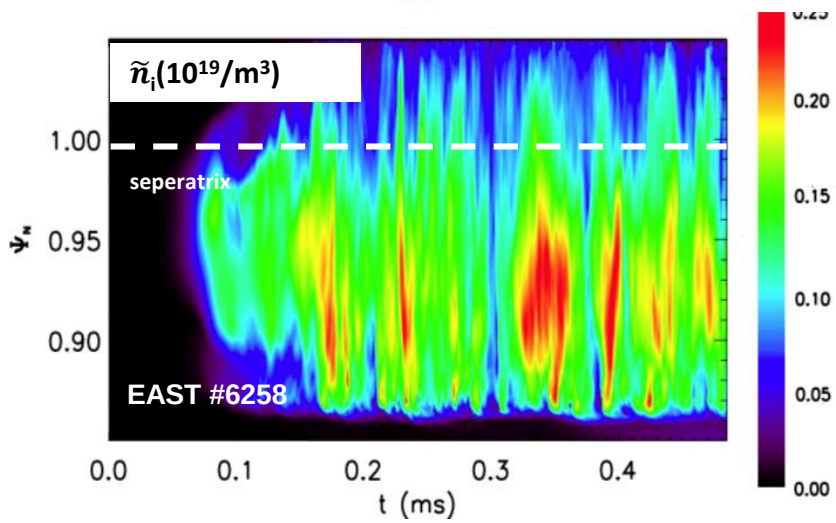


Since the multi-scale process for e^- and ions, we use both transport and turbulence code

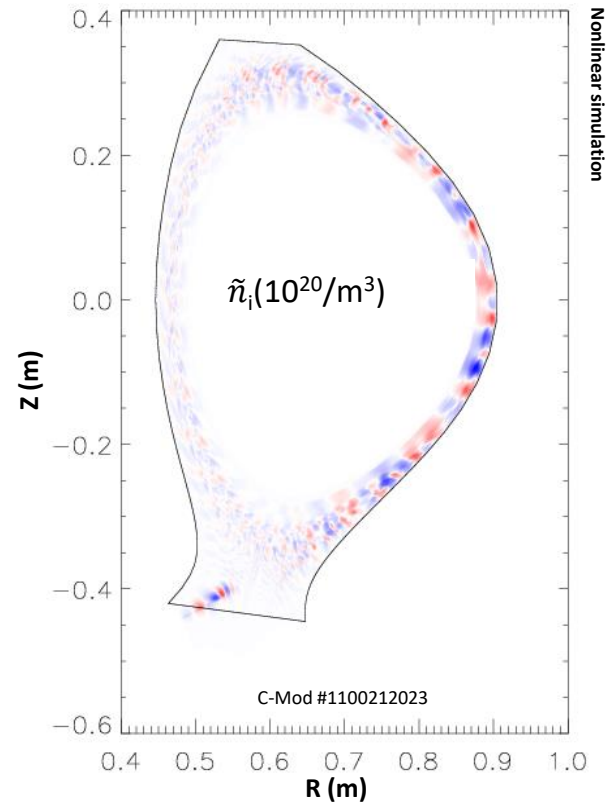
EM turbulence originates inside the pedestal near ∇P_{peak} & nonlinearly spreads across the separatrix into the SOL

Density fluctuation across separatrix at outside mid-plane





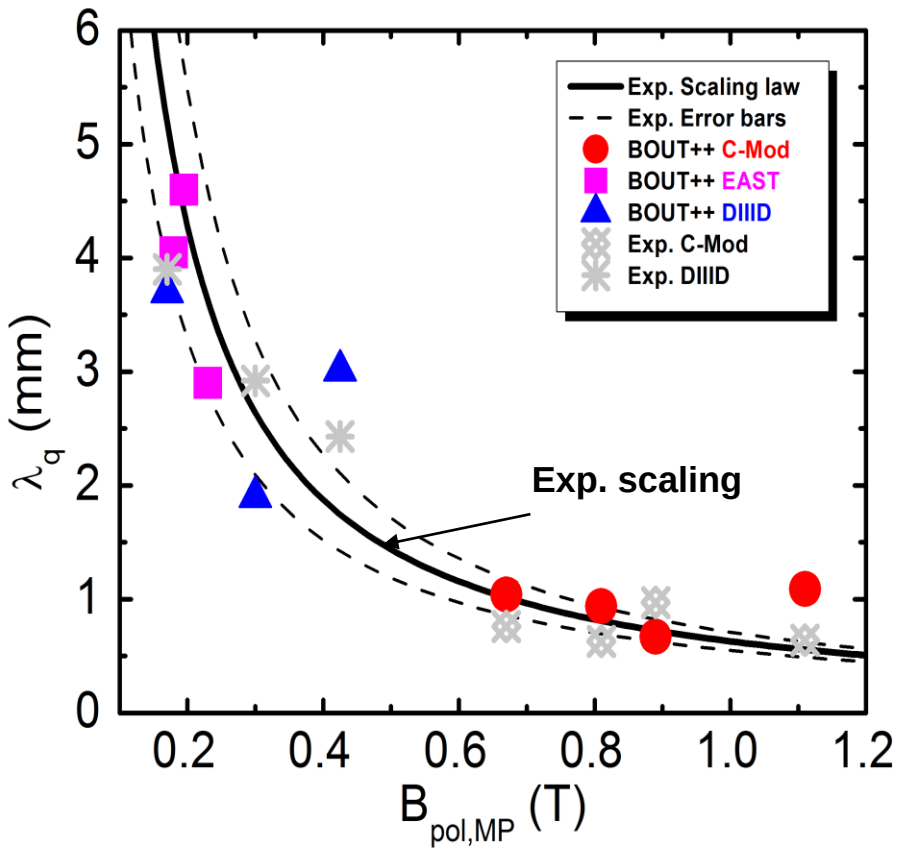
Poloidal: LFS

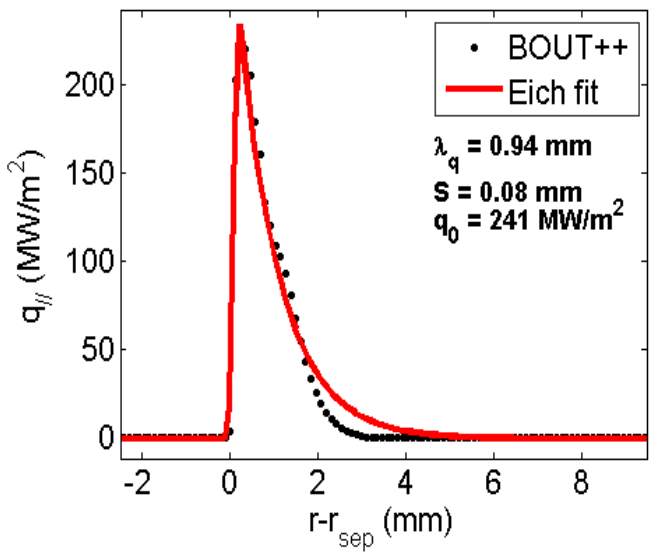


The mode structure: dominant at the LFS

The e⁻ heat flux width from BOUT++ turbulence simulations of C-Mod, DIII-D and EAST follows exp. "Eich" scaling

$$\lambda_q = 0.63 B_{pol}^{-1.19}$$



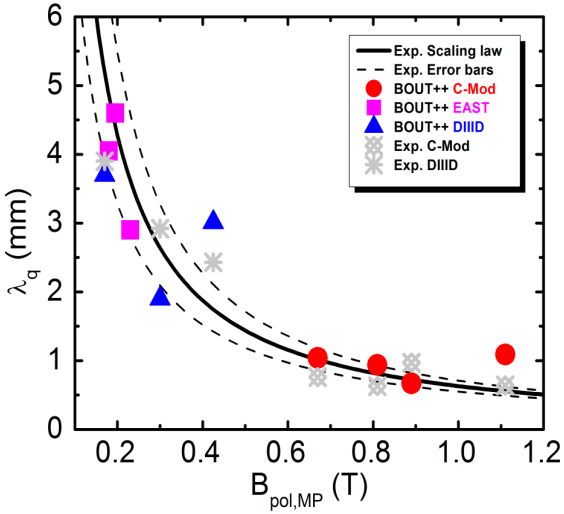


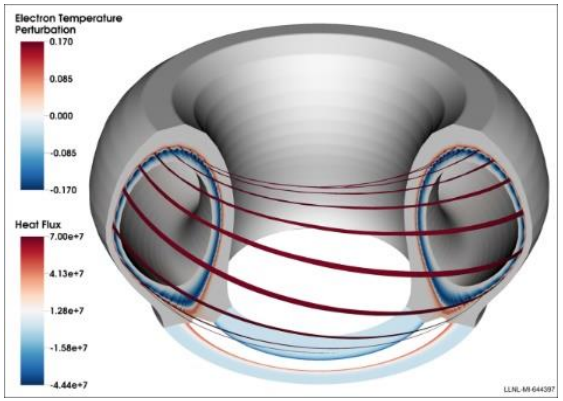
- **The amplitude of the electron heat fluxes is within a factor of 2 compared to experiment**

[1] B. Chen, X. Q. Xu, et al, Phys. Plasmas 25, 055905 (2018)
[2] T.F. Tang, et al, 2017, submitted to Phys. Plasmas;.
[3] T.Y. Xia, et al, 2017, Nucl. Fusion, 57, 116016.

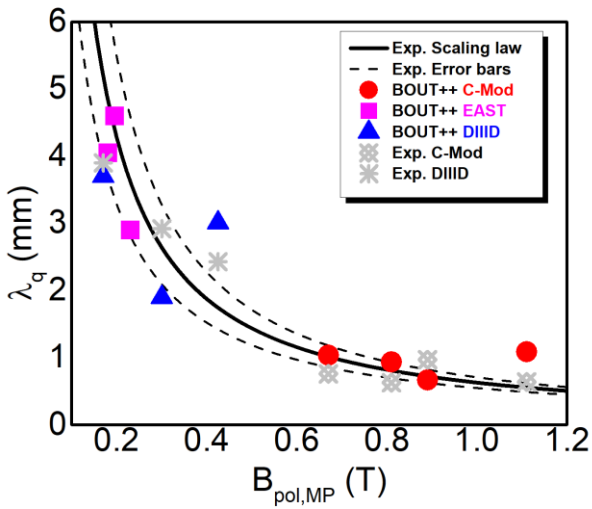
Principal Results

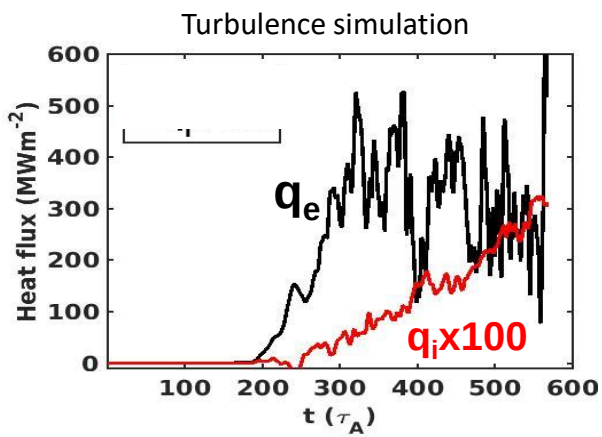
- BOUT++ turbulence code is used to simulate the electron heat flux width λ_q, which is consistent with experimental Eich scaling
  - ✓ The large SOL turbulence originates from the peak gradient region inside the pedestal and not from local instabilities in the SOL
  - ✓ Turbulence simulations compared well with data from C-Mod
- **Transport simulations show that**
  - ✓ **Drifts and turbulent transport are locked in a tight competition for C-Mod**
  - ✓ ITER & CFETR will possibly be in a turbulence dominant regime

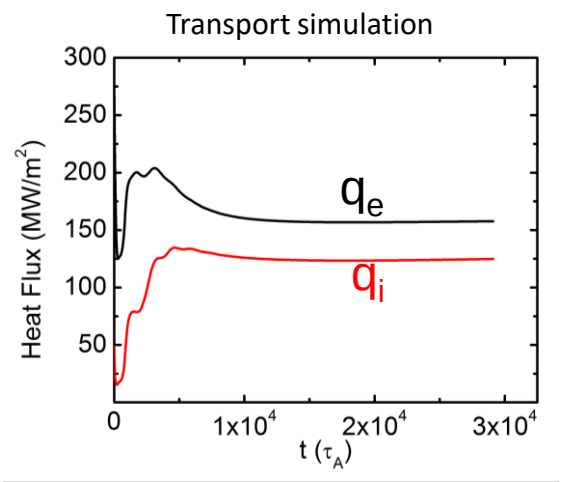




“Steady state” heat flux is obtained from BOUT++ transport simulation for both ion and electron







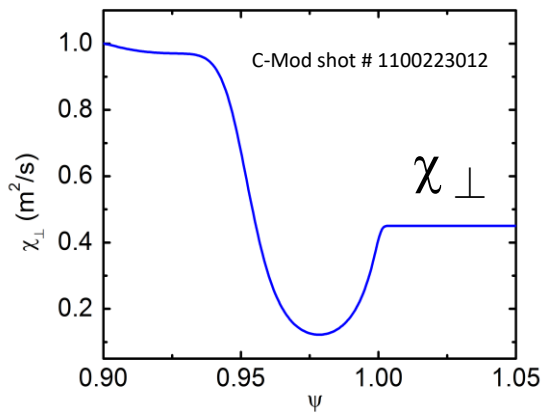
- **Electron heat flux well saturated, not easy for ions due to slower timescale of ion parallel transport [1]**
- **Developed a plasma fluid transport model with all drifts[2]:**
  - ✓ **mimic Goldston’s Heuristic drift-based model**
  - ✓ **steady state solution for both electrons and ions**

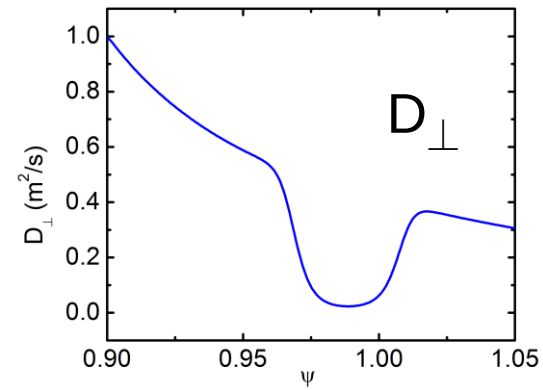
[1]B. Chen, X. Q. Xu, et al., PoP (2018)
[2] N.M. Li, , X. Q. Xu, et al., CPC (2018)

BOUT++ transport code is used to get steady state solution for both electrons and ions

- **BOUT++ 3D 6-field 2-fluid transport evolves**
  - ✓ **density n_i,**
  - ✓ **ion temperature T_i**
  - ✓ **electron temperature T_e**
  - ✓ **parallel velocity $v_{||i}$**
  - ✓ **vorticity ϖ**
  - ✓ **Ohm's law $j_{||}$ for current**

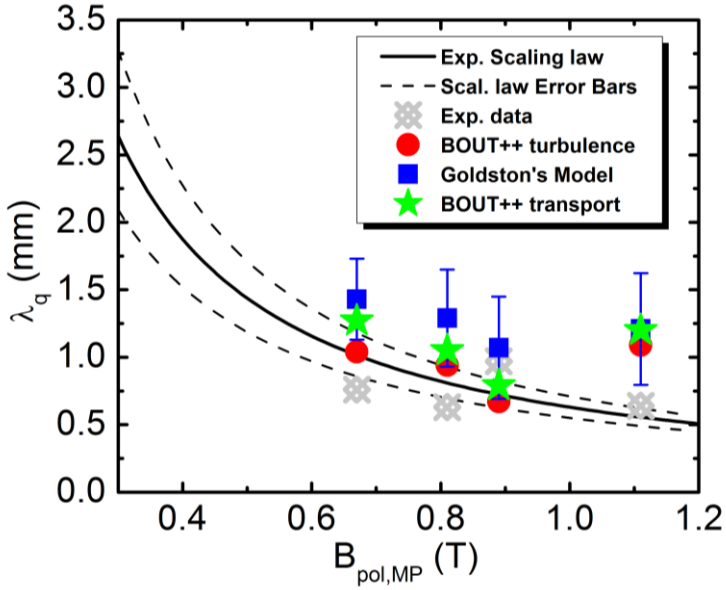
- **To simulate tokamak divertor heat flux width**
  - ✓ **Transport coef profiles inside the separatrix are prescribed in order to match the steady-state n & T profiles there**
  - ✓ **In the SOL, the value is consistent with the turbulence code calculation**





N.M. Li, X. Q. Xu, et al., CPC.(2018)

Calculated heat flux width from BOUT++ transport is similar to Goldston's model and turbulence simulations

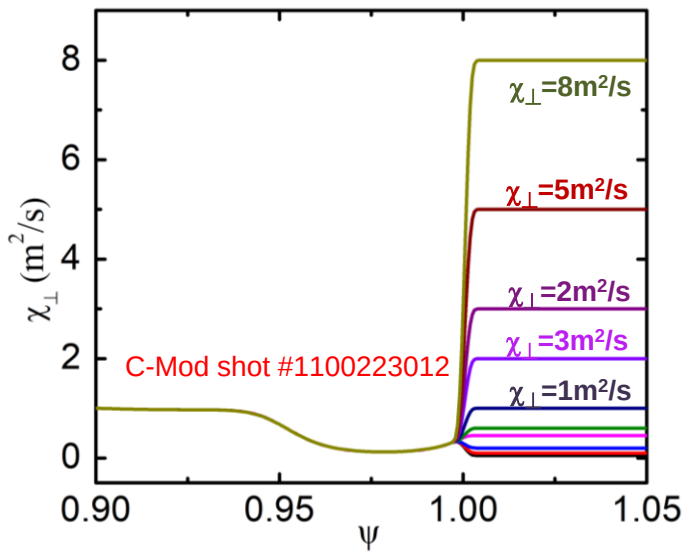


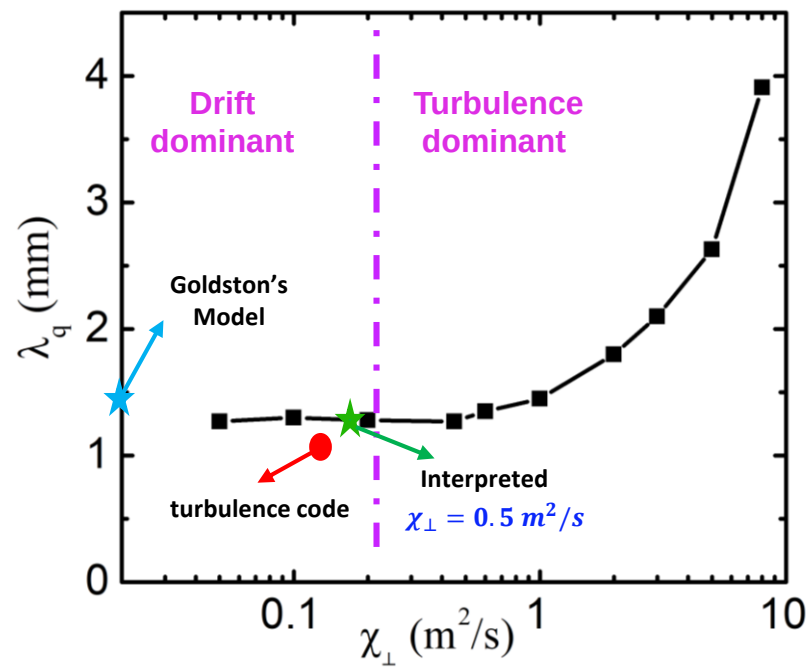
Goldston's HD formula

$$\lambda_q = \frac{4a}{\bar{Z}eB_pR}\left(\frac{\bar{A}m_pT_{sep}}{1+\bar{Z}}\right)^{1/2}$$

- **The electron and ion heat flux width on the divertor targets follow similar trends**
- **Large λ_q for B_p=1.1T is due to higher separatrix temperature measured from expt.**

The drifts and turbulent transport are locked in a tight competition in setting the divertor heat flux width for C-Mod

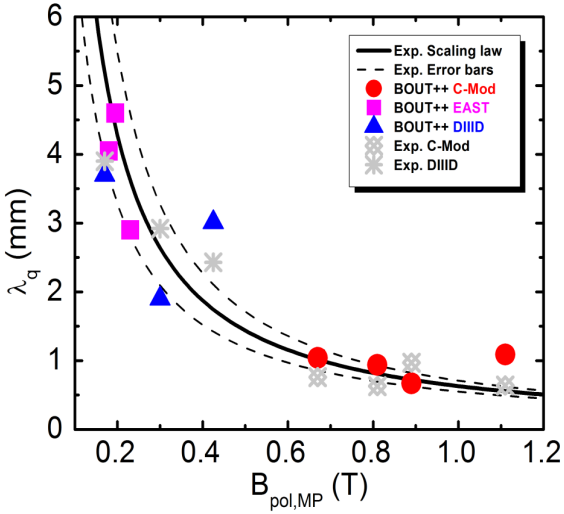


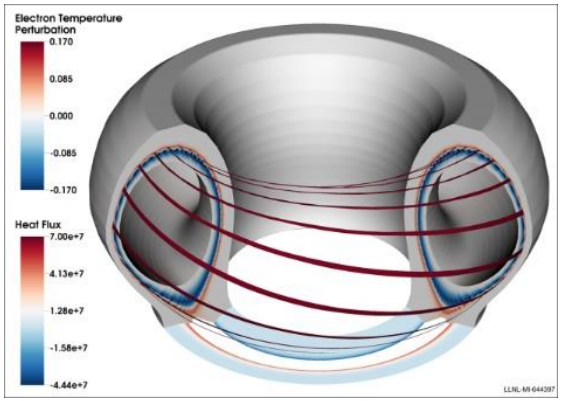


- **Heat flux width is flat and then increases with the SOL perpendicular transport coefficient**
- **$\chi_{\perp,critical}$ is found**
  - **$\chi_\perp < 0.5\ m^2/s$, drifts dominate cross-field transport**
  - **$\chi_\perp > 0.5\ m^2/s$, turbulence dominates cross-field transport**
- **Interpreted $\chi_\perp = 0.34\ m^2/s$ from experiments**
- **Calculated $\chi_\perp = 0.23\ m^2/s$ from turbulent simulations**

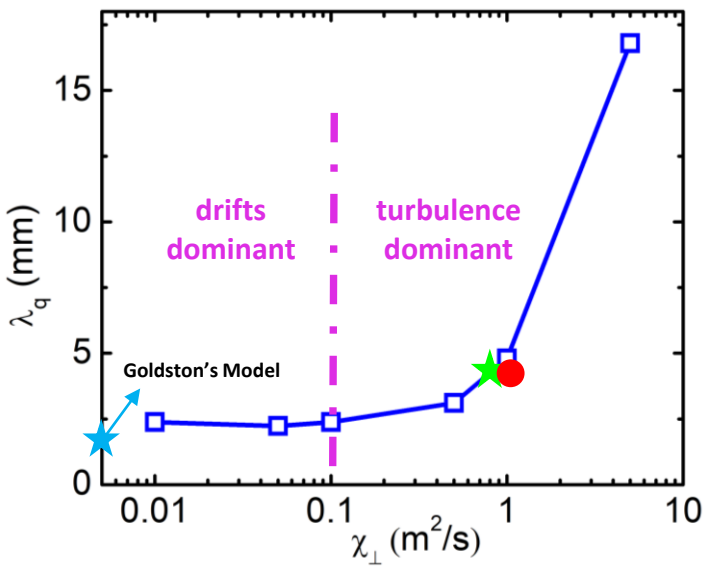
Principal Results

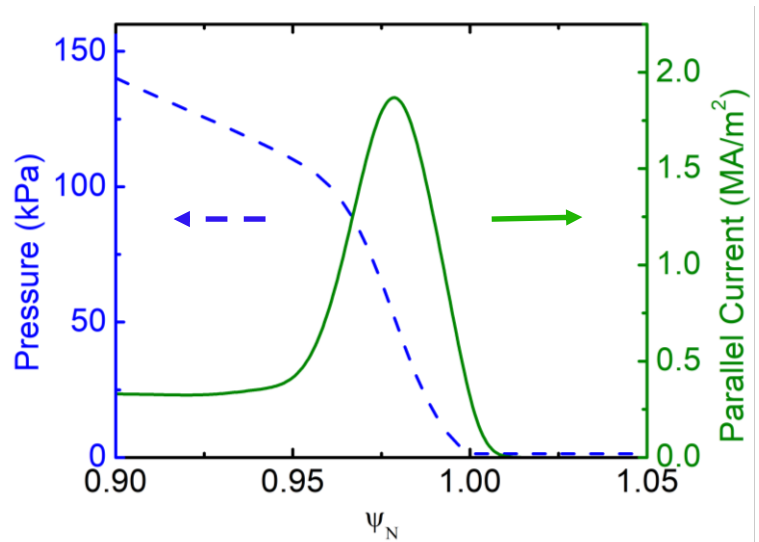
- BOUT++ turbulence code is used to simulate the electron heat flux width λ_q, which is consistent with experimental Eich scaling
  - ✓ The large SOL turbulence originates from the peak gradient region inside the pedestal and not from local instabilities in the SOL
  - ✓ Turbulence simulations compared well with data from C-Mod
- **Transport simulations show that**
  - ✓ Drifts and turbulent transport are locked in a tight competition for C-Mod
  - ✓ **ITER & CFETR will possibly be in a turbulence dominant regime**





CFETR will possibly be in a turbulent dominant regime with some drift contribution in setting divertor heat flux width

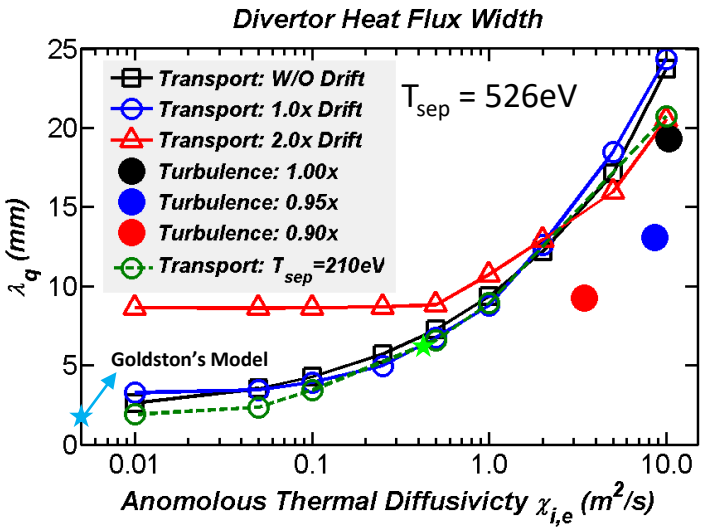


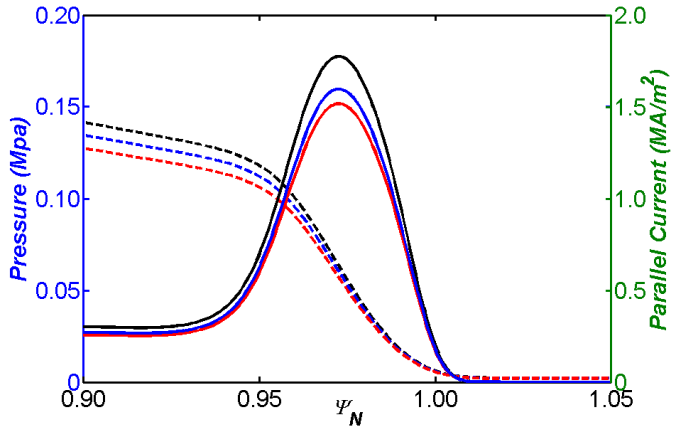


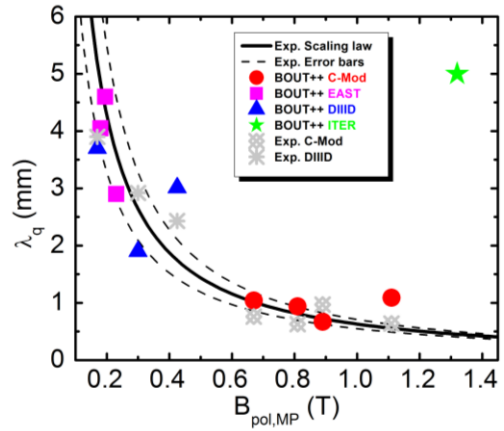
Plasma profiles from scenario studies using OMFIT

- $\chi_{\perp,critical}$ **is found**
  - ✓ $\chi_\perp < 0.1\ m^2/s$, **drifts dominant**
  - ✓ $\chi_\perp > 0.1\ m^2/s$, **turbulence dominant**
- **HD model sets the lower limit of divertor heat flux width**
- **Interpreted $\chi_\perp = 0.85\ m^2/s$ from Plasma profiles in scenario studies**
- **Grassy ELMs → larger $\chi_\perp$ & λ_q, better for high-performance steady-state operations**

High ITER pedestal pressure leads to large transport & wide divertor heat flux width





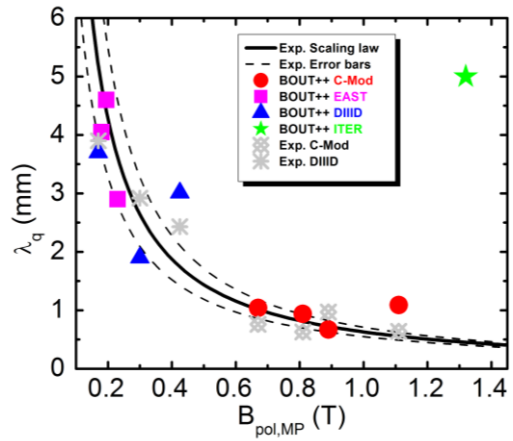


[1] S.H. Kim et al. "Simulating Burning Plasma Operation in ITER", EPS, Lisbon, 2015

- **Plasma profiles from scenario studies using CORSICA [1]**
- **HD model sets the lower limit of divertor heat flux width**
- **Drift becomes sub-dominant in ITER simulation due to large R**
- **Turbulent transport coefficients depend on pedestal structures inside the separatrix**
- **Interpreted $\chi_\perp = 0.3\ m^2/s$ from Plasma profiles in scenario studies**
- **λ_q no longer follows the $1/B_{pol,MP}$ experimental Eich scaling law**

Principal Results

- **BOUT++ turbulence code is used to simulate the electron heat flux width λ_q, which is consistent with experimental Eich scaling**
  - ✓ **The large SOL turbulence originates from the peak gradient region inside the pedestal**
  - ✓ **Turbulence simulations compared well with data from C-Mod**



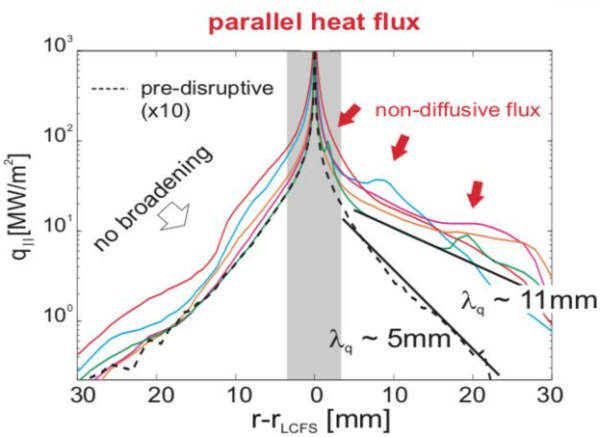
- **Transport simulations show that**
  - ✓ **Drifts and turbulence are locked in a tight competition for C-Mod**
    - **$\chi_{\perp,critical}$ is found**
  - ✓ **ITER & CFETR will possibly be in a turbulence dominant regime**
    - **HD model sets the lower limit of divertor heat flux width λ_q**
    - **λ_q is no longer size independent**
    - **λ_q no longer follows the $1/B_{pol,MP}$ experimental Eich scaling law**

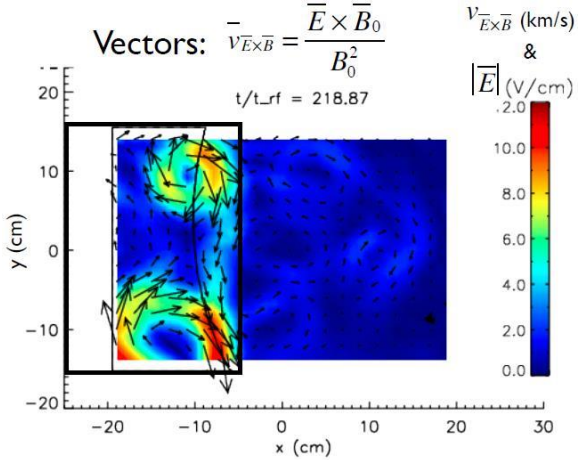
- **Grassy ELMs → larger $\chi_\perp$ & λ_q**

The best compromise between divertor solutions and high-performance steady-state operations

Future Opportunities

- **Tokamak Disruption Simulations**
  Develop simulation capabilities to understand two salient features on the power exhaust to the divertor plates
  - Significant scrape-of-layer broadening, in the range of 5-20.
  - The core temperature collapses in τ_{TQ}~1 ms, the peak thermal load arriving at the divertor is spread over a longer time period τ_d. On JET, for density limited disruptions, τ_d/τ_{TQ} is observed to be 3-8.
- **Plasma – RF interactions**
  - RF sheaths and ponderomotive forces driven shear flows
  - Modification of the SOL turbulence profiles via RF driven flow
  - RF propagation is impacted by the SOL turbulence
- **Plasma – material interactions**
  - Determine the importance of intermittent transient events such as ELMs on impurity production and material erosion
  - Understand how plasma turbulence impacts the dynamic recycling of main ions and impurities between the plasma & material surfaces
- **Whole device Modelling**
  - Provide a GYRO-Landau-Fluid solver for turbulence-driven anomalous transport in SOL

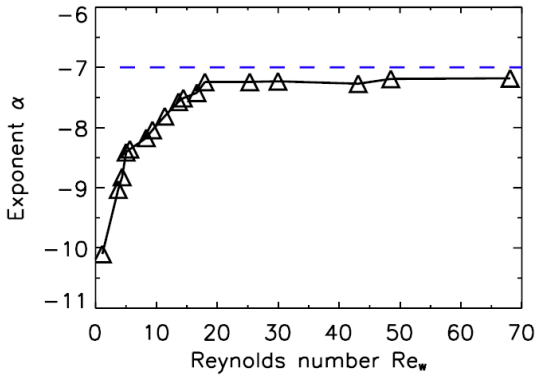




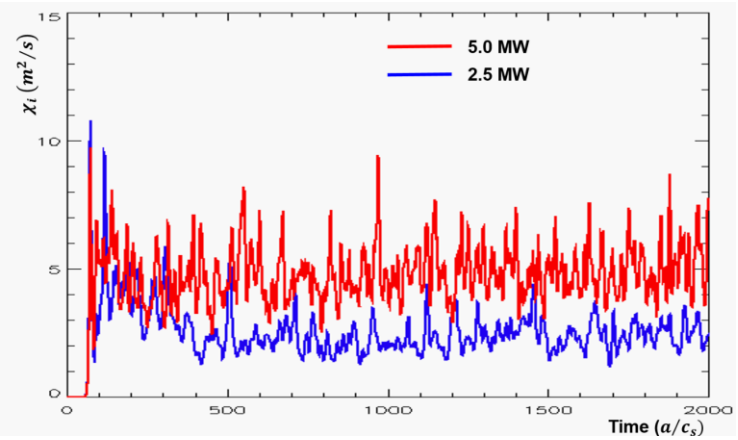
Backup slides

Research at NFRI (Korea) using BOUT++

- **Fundamental study of plasma turbulence using simple model**
  - ➢ **Determination of inertial range exponent in Hasegawa-Mima turbulence**
  - ➢ **Impact of parallel compressions on zonal flow pattern formation**

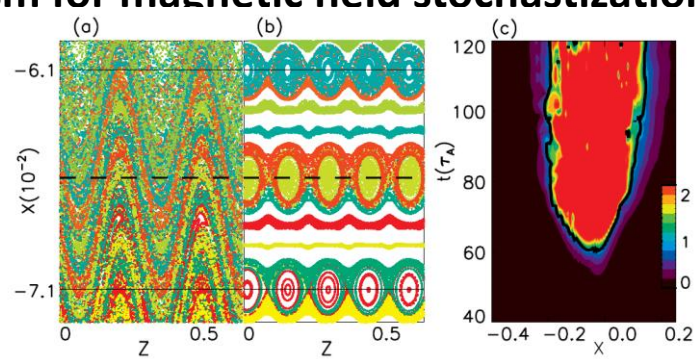


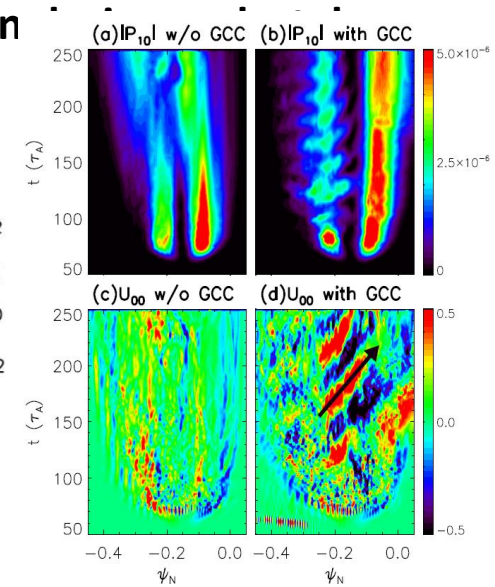
- **Physics of core ion temperature gradient (ITG) turbulence**
  - ➢ **Global flux-driven reduced 3+1 model**
  - ➢ **Global 4+2 model development on-going**



Research at NFRI (Korea) using BOUT++

- **In-depth analysis of nonlinear stage of pedestal collapse**
  - **Elucidation of the mechanism for magnetic field stochastization**
  - **collapse**
  - **Impact of n=0 GAMs**
  - **Impact of RMP on-going**





- **Linear/quasi-linear analyses of**
  - **Electromagentic effects on intrinsic rotation generation**
  - **Physics of plasma response to RMP**