Latest developments in BOUT++ boundary plasma turbulent transport simulations

2023 BOUT++ workshop
9-12 January 2023, Livermore, CA, USA

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In collaboration with BOUT++ team

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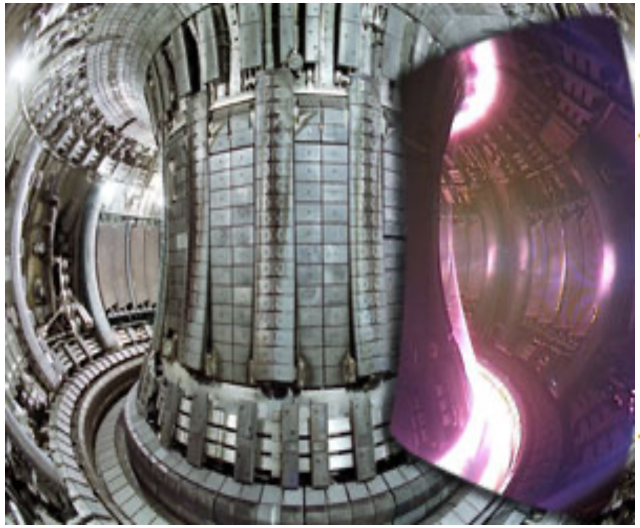
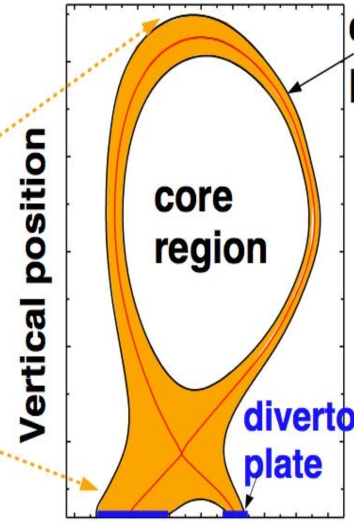
Lawrence Livermore National Laboratory

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





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

- ✓ **Accelerating with GPU**
- ✓ **Multiscale simulations**
- ✓ **Full annular tokamak edge**
- ✓ **Multi-ion models**
- ✓ **Neutrals & Impurities**
- ✓ **Flux-driven simulations**
- ✓ **ITER & FPP**

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

2000 | 2005 | 2009 | 2023

- *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++ have been products of broad international collaborations

Soochow University

UKRI Science and Technology Facilities Council

Hartree Centre

IFS Theory Group, Institute for Fusion Studies

Delhi Technological University (DelTech)

The University of California (UCLA)

UCSD

General Atomics

Argonne National Laboratory

Illinois Institute of Technology

MEPhI – National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

The University of Edinburgh

DCU

CCFE – Culham Centre for Fusion Energy

University of York

Berkeley Lab – Lawrence Berkeley National Laboratory

MIT PSFC

IPP Max-Planck-Institut für Plasmaphysik

William & Mary

QST

TECH-X

Lodestar Research Corporation

Lawrence Livermore National Laboratory

HIT

Huazhong University of Science & Technology

Frazer-Nash Consultancy – A KBR Company

Oak Ridge National Laboratory

Norges Arktiske Universitet – UiT

POSTECH 포항공과대학교

UNIST

Xihua University

Sichuan University

University of Science and Technology of China

西安交通大學 Xi'an Jiaotong University

Southwest Jiaotong University

KFE

NFRI 국가핵융합연구소 National Fusion Research Institute

Soongsil University 1897

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

SWIP Southwestern Institute of Physics

Dalian University of Technology

Institute of plasma Physics Chinese Academy of Sciences

The University of Wisconsin Madison

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

Multiple Institutions (> 40) around the globe join BOUT++ developments and applications

- **USA**

LLNL, GA, UCSD, MIT, UW Madison, UCLA, Tech-X, Lodestar, LBNL, ANL, …

- **Europe**

U York, CCFE, DTU, DCU,…

- **Asian**

  - **China**

ASIPP, Peking U, DLUT, USTC, SWIP, Zhejiang U. HUST, SCU, SWJTU, XJTU, XHU, HIT,…

  - **Japan**

QST-Rakkasho

  - **Korea**

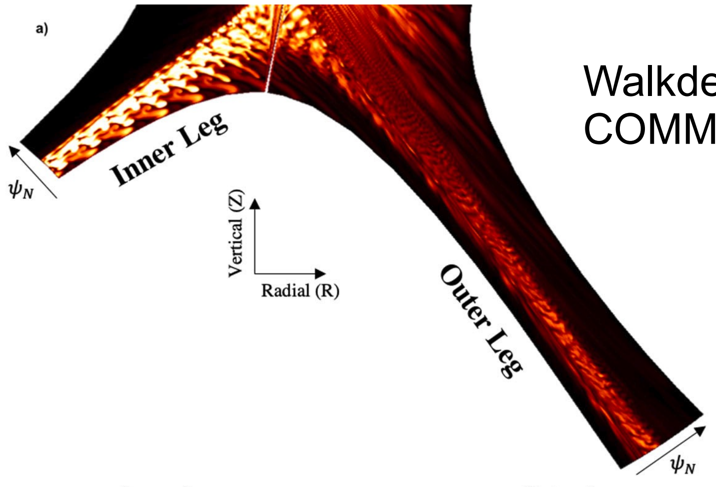
NFRI, POSTECH, UNIST, Soongsil University,…

BOUT & BOUT++ Work Produced Multiple Publications since 2018

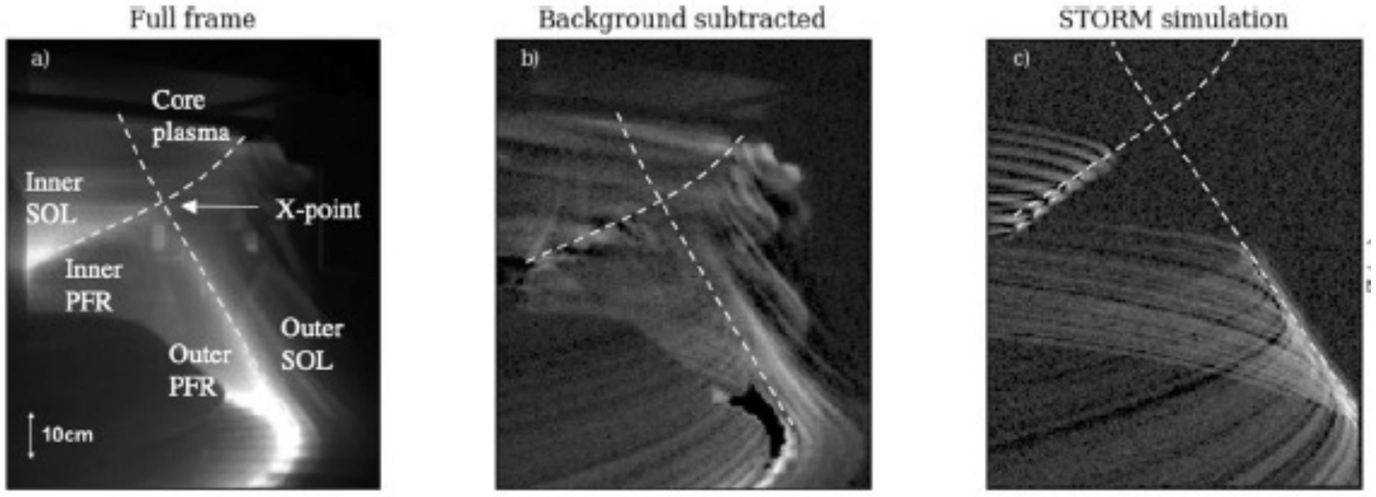
- **Journal Publications, >109**
  - ✓ NATURE COMMUNICATIONS PHYSICS
  - ✓ PRL
  - ✓ Nuclear Fusion
  - ✓ JCP
  - ✓ CPC
  - ✓ PoP
  - ✓ PPCF
  - ✓ JNE
  - ✓ Science China Physics, Mechanics & Astronomy
  - ….

https://bout.llnl.gov/publications

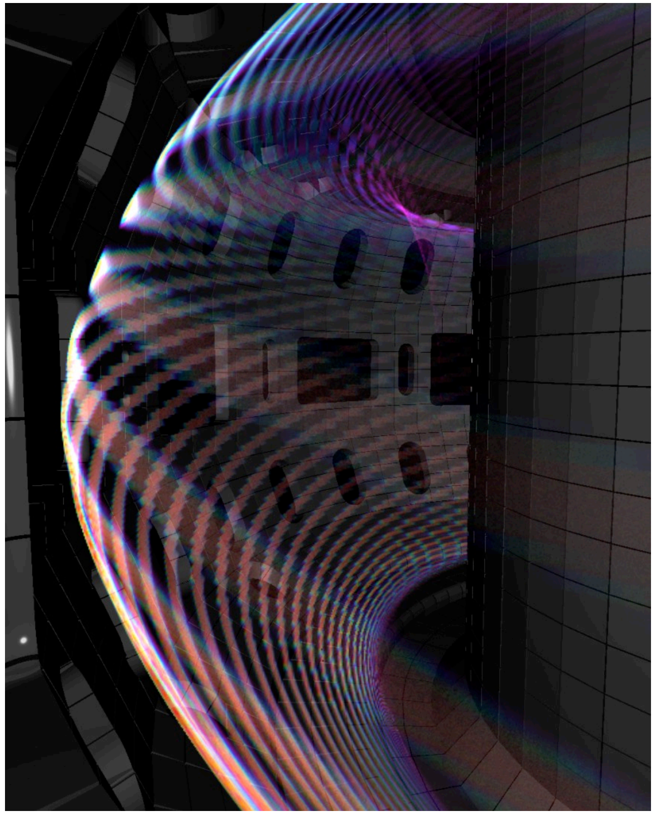
http://boutproject.github.io/publications/



Walkden, et al. 2022, COMMUNICATIONS PHYSICS



Principal Results since 2018 BOUT++ workshop



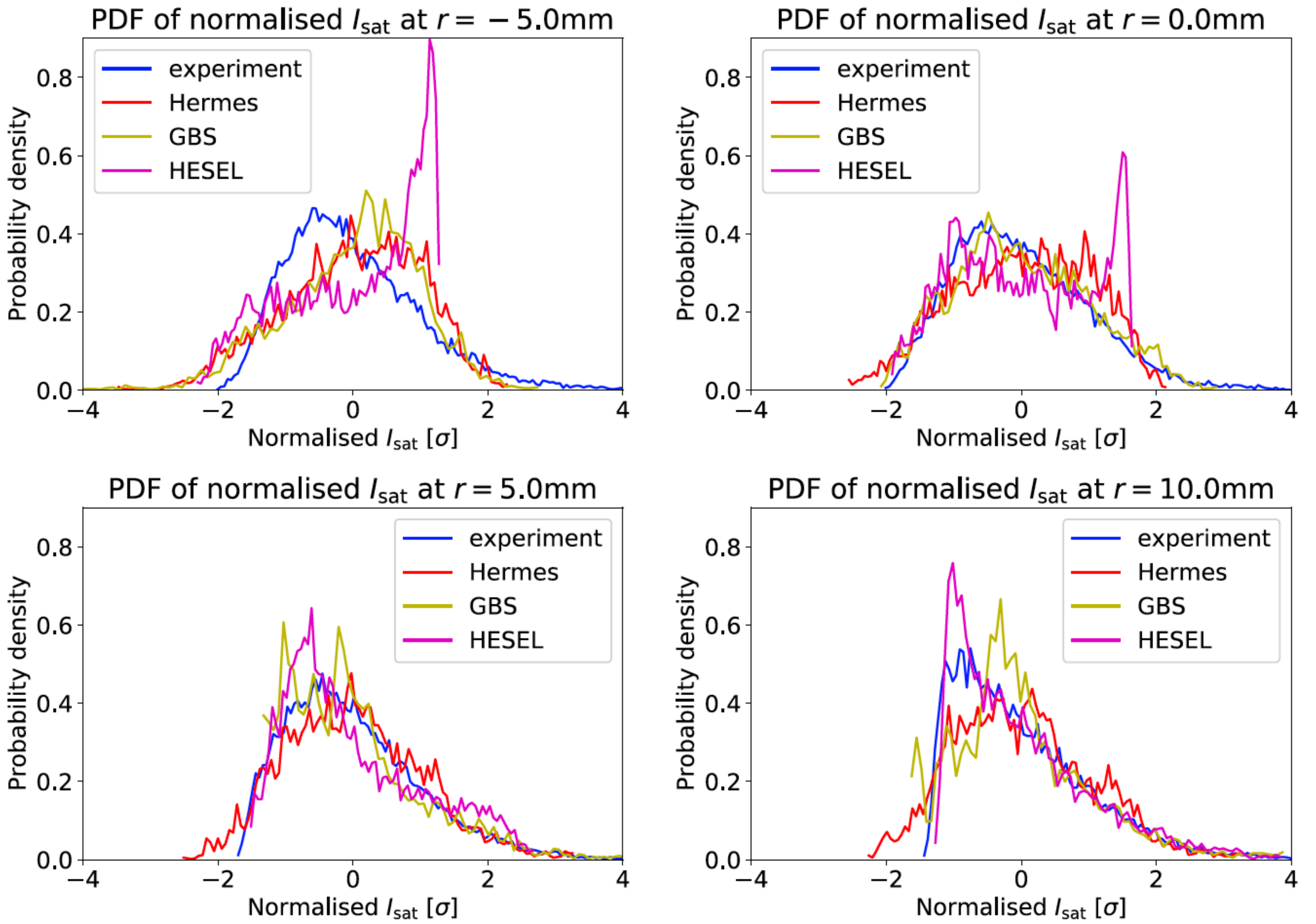
- Formulation / Theory
  - Landau Fluid Closures
  - Micro-tearing

- Code Development
  - Accelerating BOUT++ with GPUs
  - SOLT3D
  - Complex meshing for Snowflake & Stellarator
  - 2D transport with drifts
  - Hermes-3
  - STORM

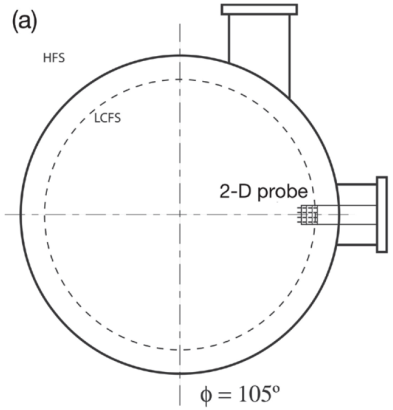
- Physics Highlights
  - Verification & Validation
  - Divertor heat flux width
  - Landau Fluid in divertor geometry
  - Extension for Full Annular Tokamak Edge
  - RF-Plasma Interactions
  - Pellet injection
  - RMP
  - Impurity and Dust Transport
  - Accelerating Multiscale Simulations with ML techniques

Edge turbulence in ISTTOK: a multi-code fluid validation

B D Dudson et al, PPCF 63 (2021) 055013

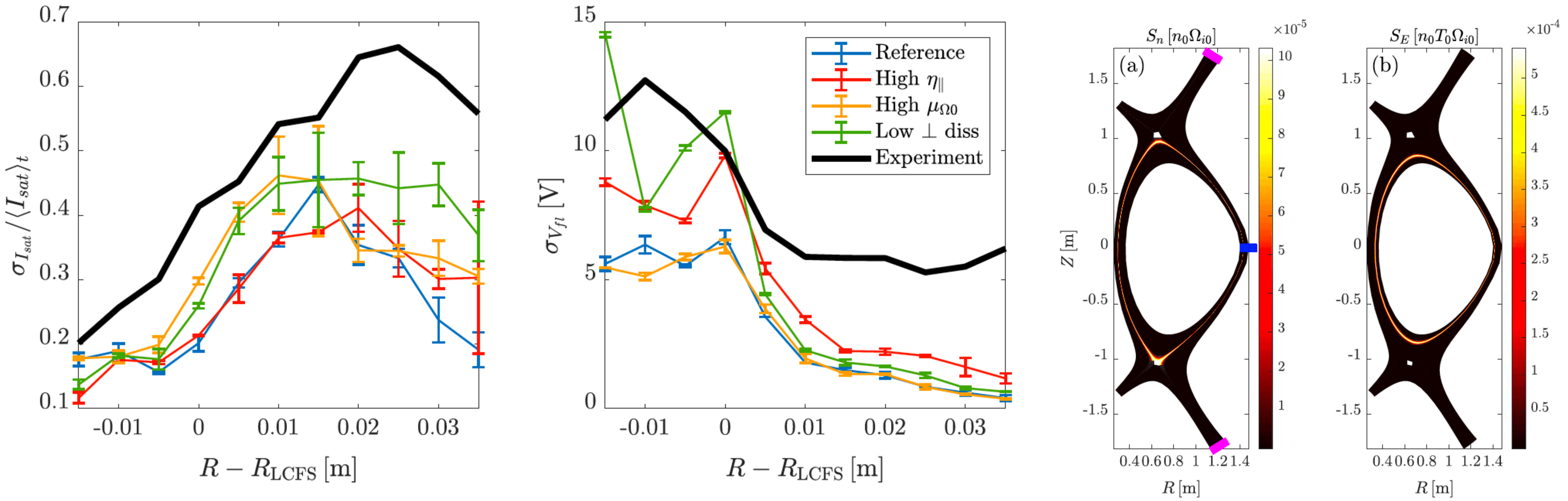


- **Undertaken through the framework of EUROfusion Enabling Research**
- **ISTTOK tokamak is a large aspect-ratio circular cross section tokamak with a poloidal graphite limiter**
- **Hermes: 3D 5-field (cold-ion) model**
- **3 Fluid codes can replicate most of the experiments in terms of I_{sat} fluctuation**



3D STORM turbulence simulations of the MAST and comparison with experimental measurements

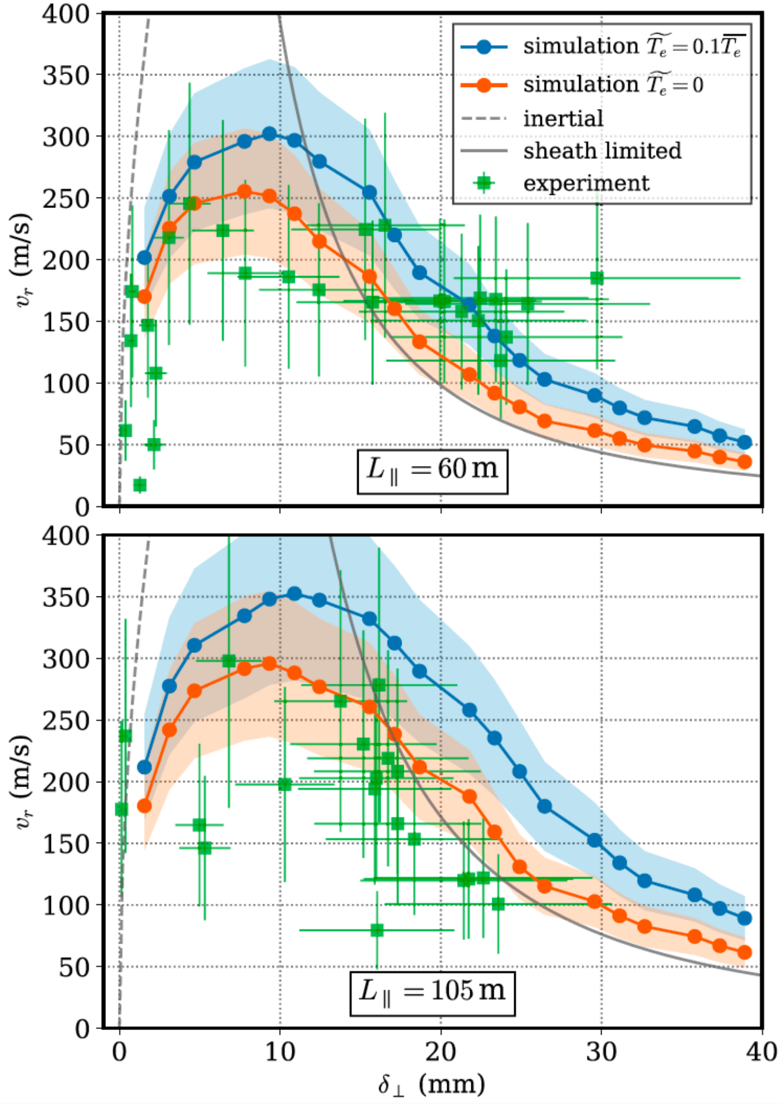
Riva, Militello, et al, PPCF 61 (2019) 095013



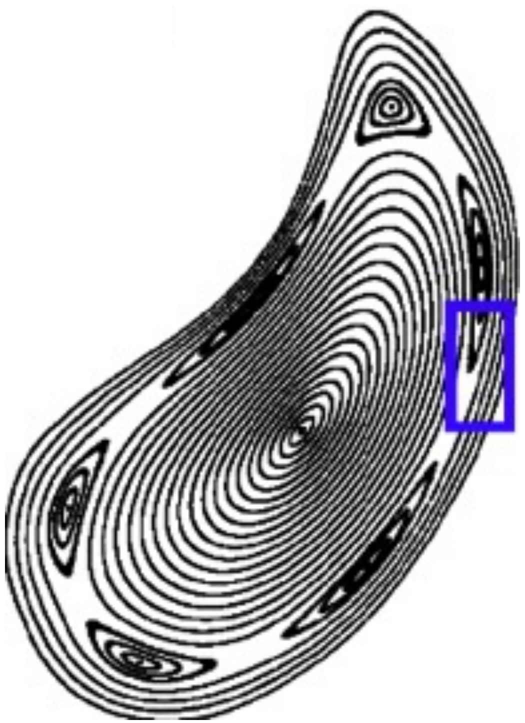
- The trends in the experiment are well captured by the simulations, with relative I_{sat} fluctuations increasing and V_{fl} fluctuations decreasing as we move radially outwards
- The simulations underestimate the amplitude of the fluctuations, both for I_{sat} and V_{fl}.

Plasma filaments in the scrape-off layer of Wendelstein 7-X

Killer, Shanahan et al, PPCF 62 (2020) 085003



- **2D simulations of seeded filaments using the Hermes model**
- **Good quantitative agreement with experimental measurements in filament velocity scalings**
- **The experiments agree better with simulations without initial Te perturbation**
- **The agreement between experiment and simulation is robust to changes in the initial Te conditions for the simulated filaments**

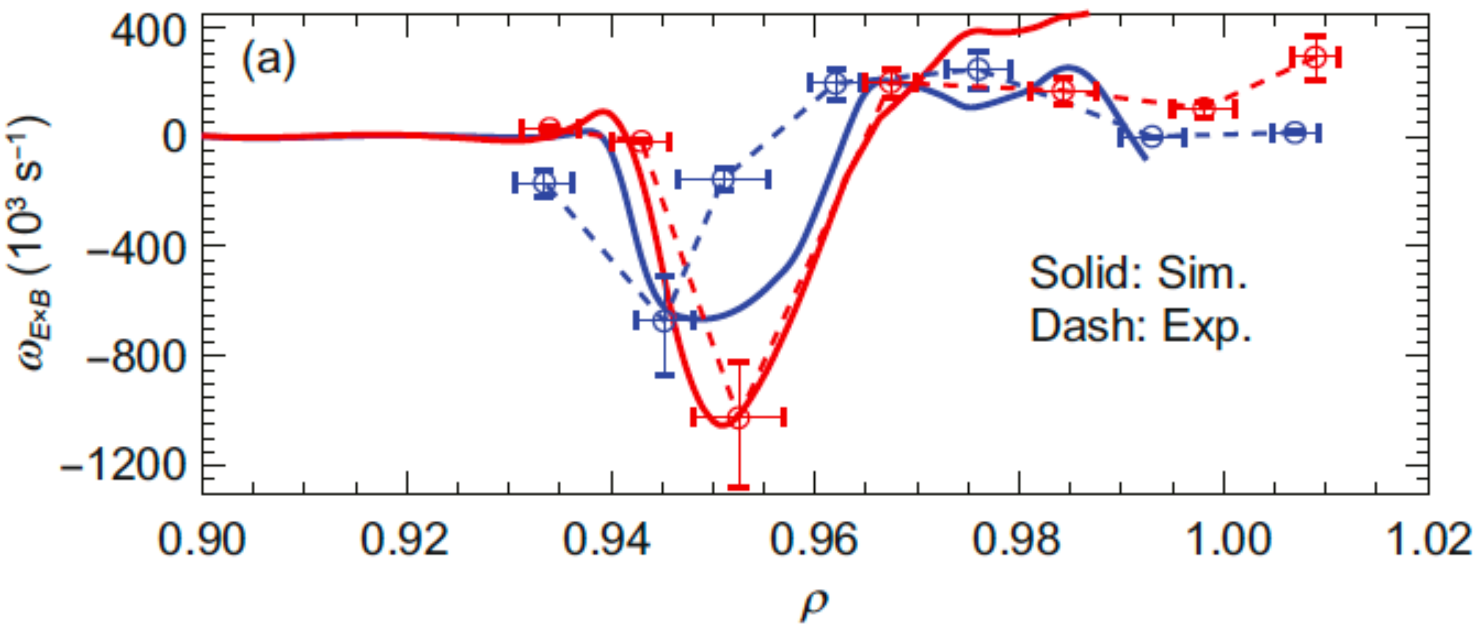


Comparison of filament scaling in experiment and simulation. The experimental data points were distinguished by connection length and simulations were performed for each connection length separately. The shaded region around the simulations results represents the uncertainty due to perpendicular filament ellipticity.

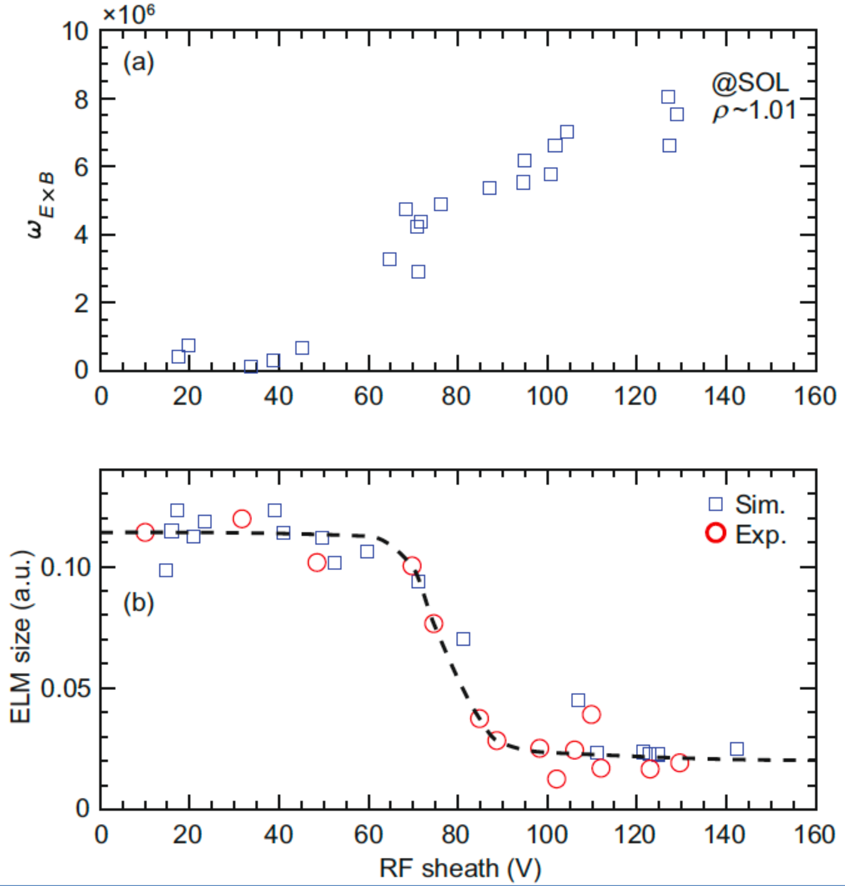
Edge localized modes suppression via edge ExB velocity shear induced by RF sheath of ion cyclotron resonance heating in EAST

XinJun Zhang, et al, SCIENCE CHINA Physics, Mechanics & Astronomy, March 2022 Vol. 65 No. 3: 235211

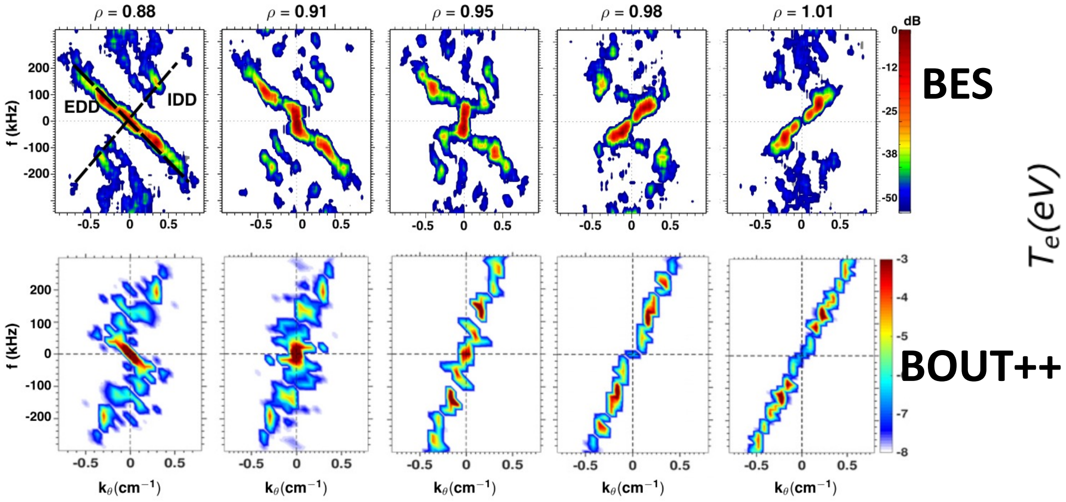
ExB frequency at the outside mid-plane before ICRH (blue curves) and during ICRH (red curves). The solid curves and dashed lines are for simulation and experiment, respectively.

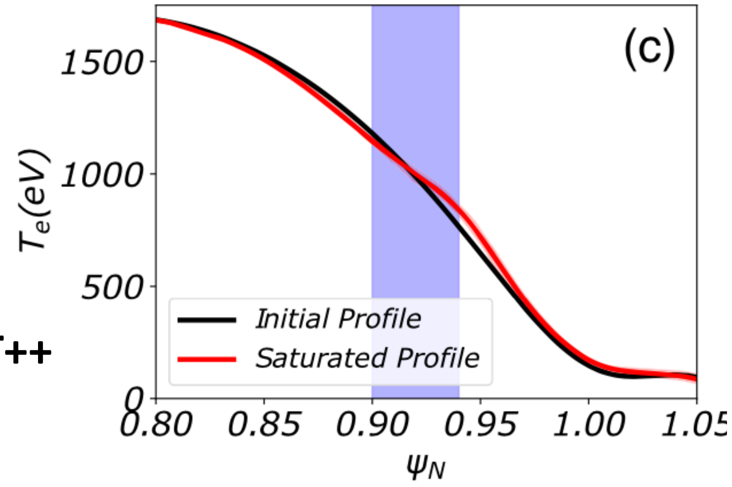


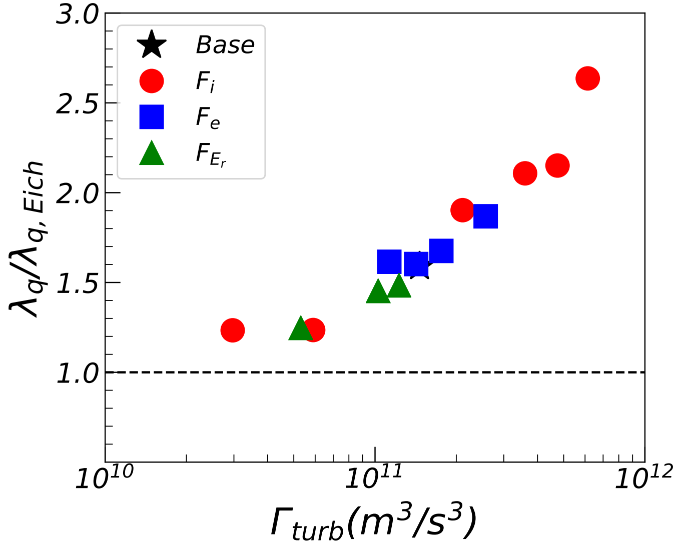
Relationship between the ExB shear rate at SOL and RF sheath potential in experiments (a) and the ELM size versus RF sheath potential from simulations and experiments in EAST (b).



The underlying physics of DIII-D newly discovered wide-pedestal QH-mode is investigated using BOUT++





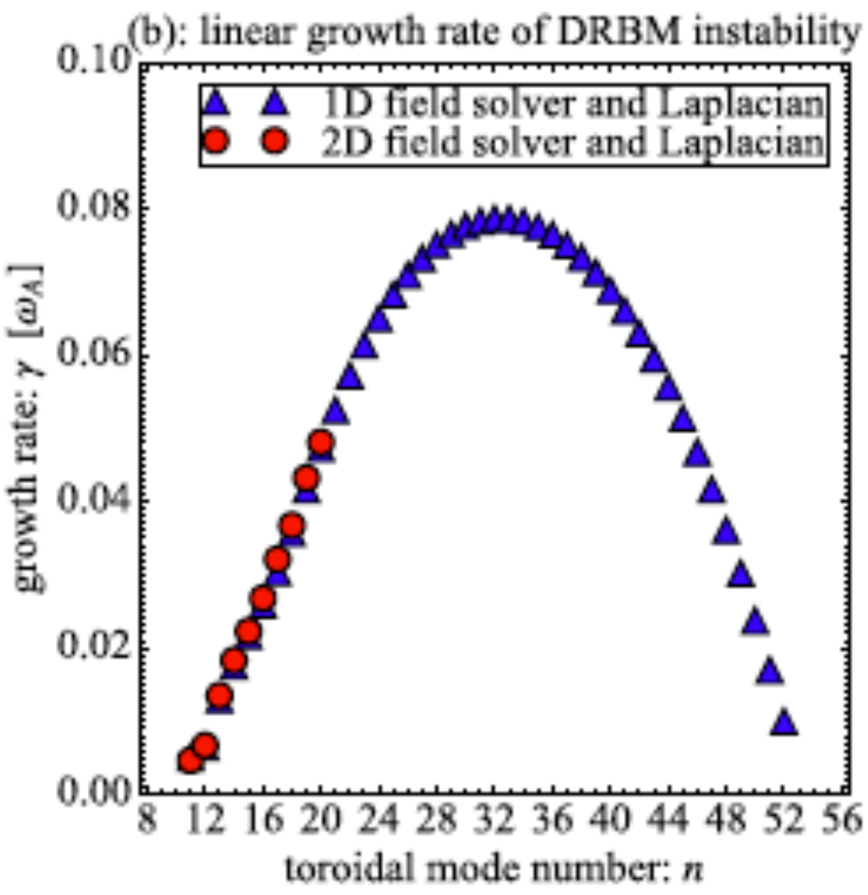


- Wide-pedestal QH-mode is newly observed in DIII-D
- The multi-scale MHD/turbulence are identified[1]
  - Large-scale, low-frequency peeing-ballooning mode
  - Small-scale, high-frequency drift Alfvén wave
- The flat-spot structure is successfully reproduced[1]
- The experimentally observed wider divertor heat flux width in WPQHM is studied[2]
  - Broadened by the large-scale mode and correlates with turbulence energy flux

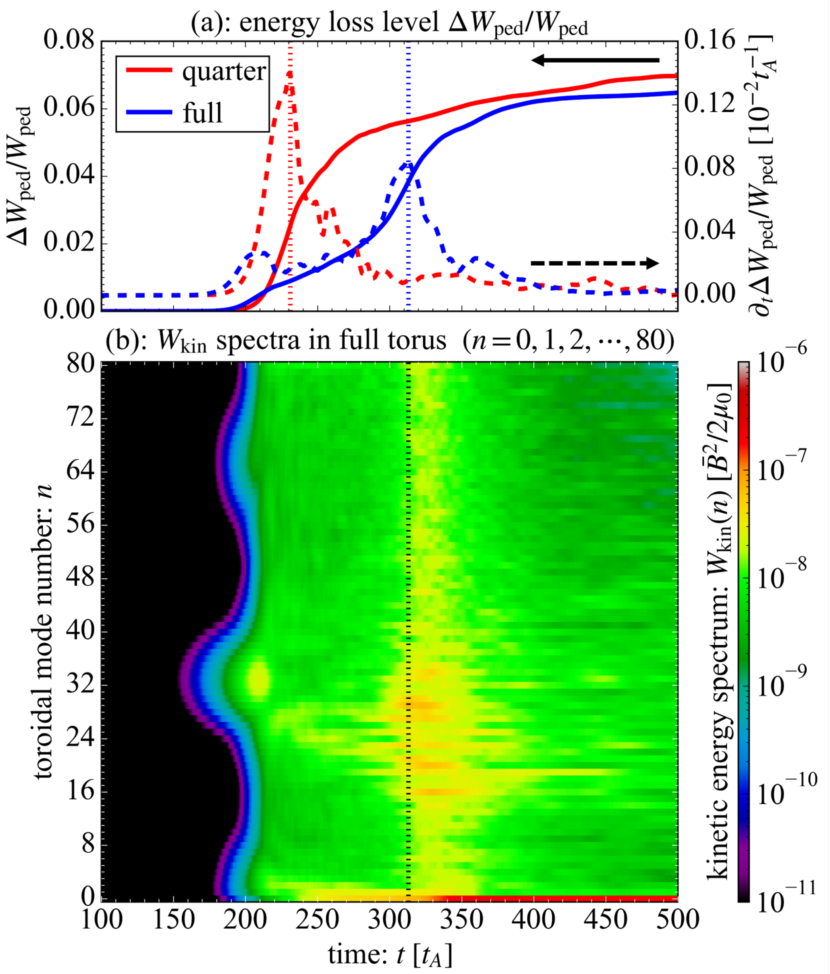
[1] Zeyu Li et al., NF 2022
[2] Zeyu Li et al., in preparation

A BOUT++ extension for full annular tokamak edge MHD and turbulence simulations

Haruki Seto, et al, Computer Physics Communications 283 (2023) 108568



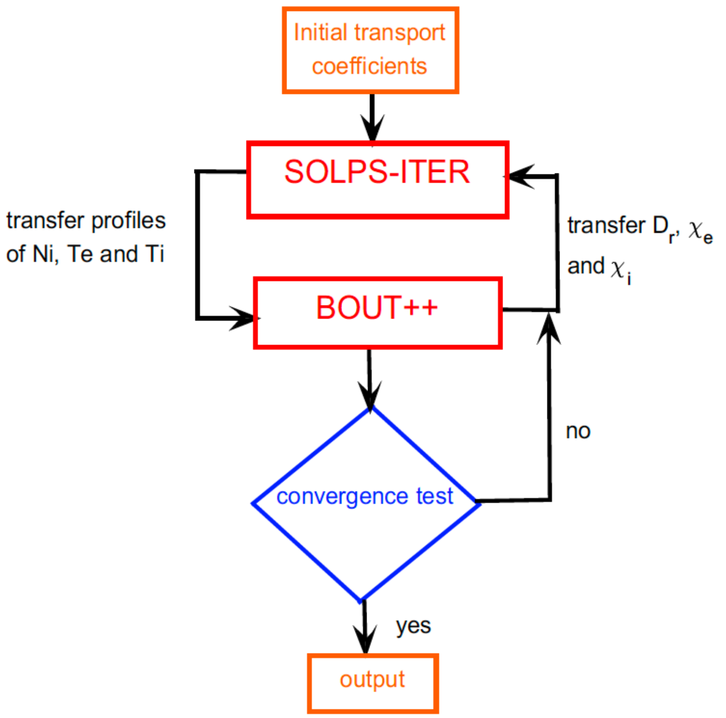
- Extended to simulate the interplay between *n* =0, low-*n* and high-*n* plasma components in a full annular tokamak edge domain through hybrid modeling of the flow potential and the vorticity
- Low-*n* modes of flow potential are calculated in an orthogonal flux surface coordinate and high-*n* modes in the dual coordinate system separately in Fourier space
- The proposed scheme can capture an interplay between *n* =1 global modes and high-*n* turbulence during pedestal collapse in a full annular torus domain with a circular cross section



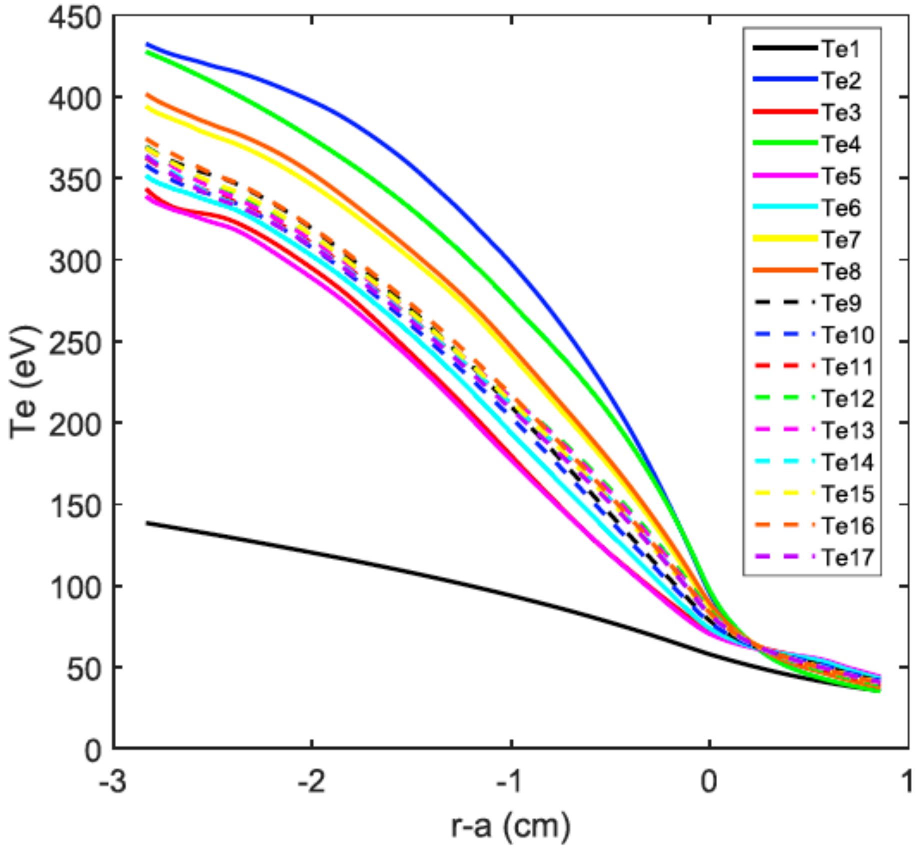
Simulation of EAST edge plasma using SOLPS-ITER/BOUT++ coupling

D.R. Zhang et al 2020 Nucl. Fusion 60 106015; Phys. Plasmas 26, 012508 (2019)

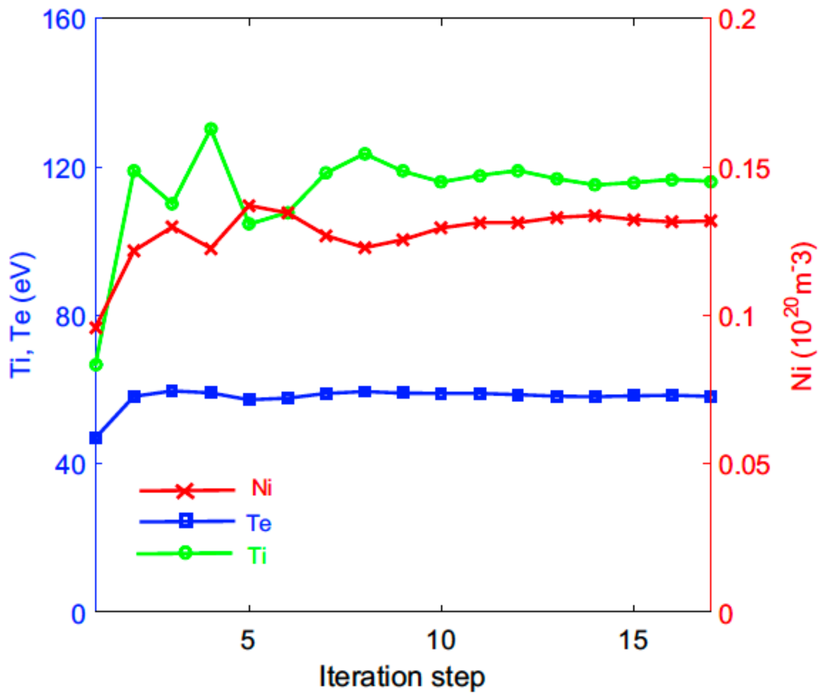
The schematic of the SOLPS-ITER/BOUT++ coupling algorithm



Te profile at outer mid-plane in iteration history. Different color and type curves represent the profiles at different iteration steps

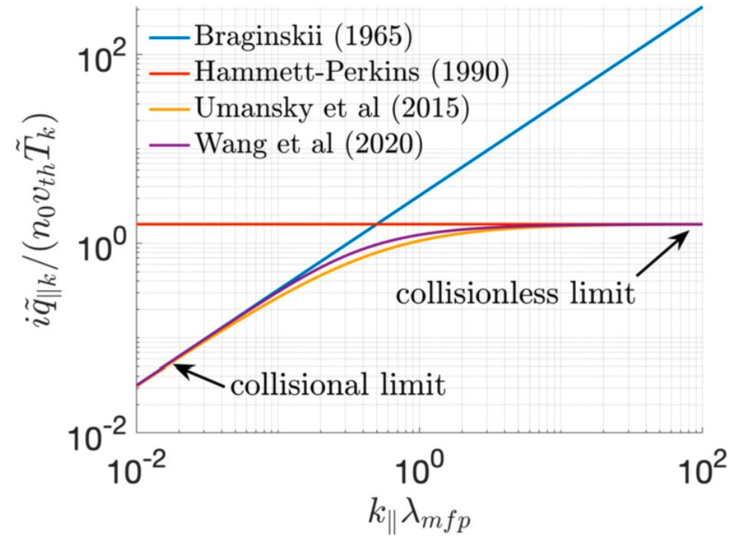


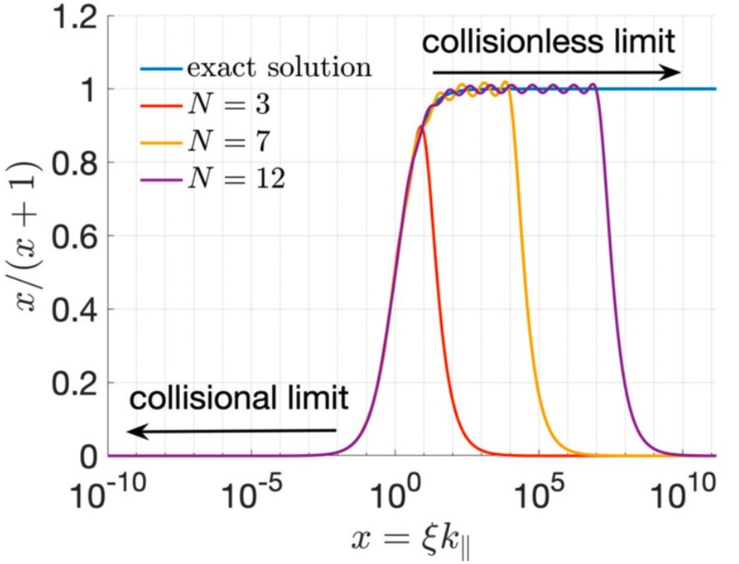
Variation of Ni, Te, Ti with iteration steps at outer mid-plane at ψ_N=1.008

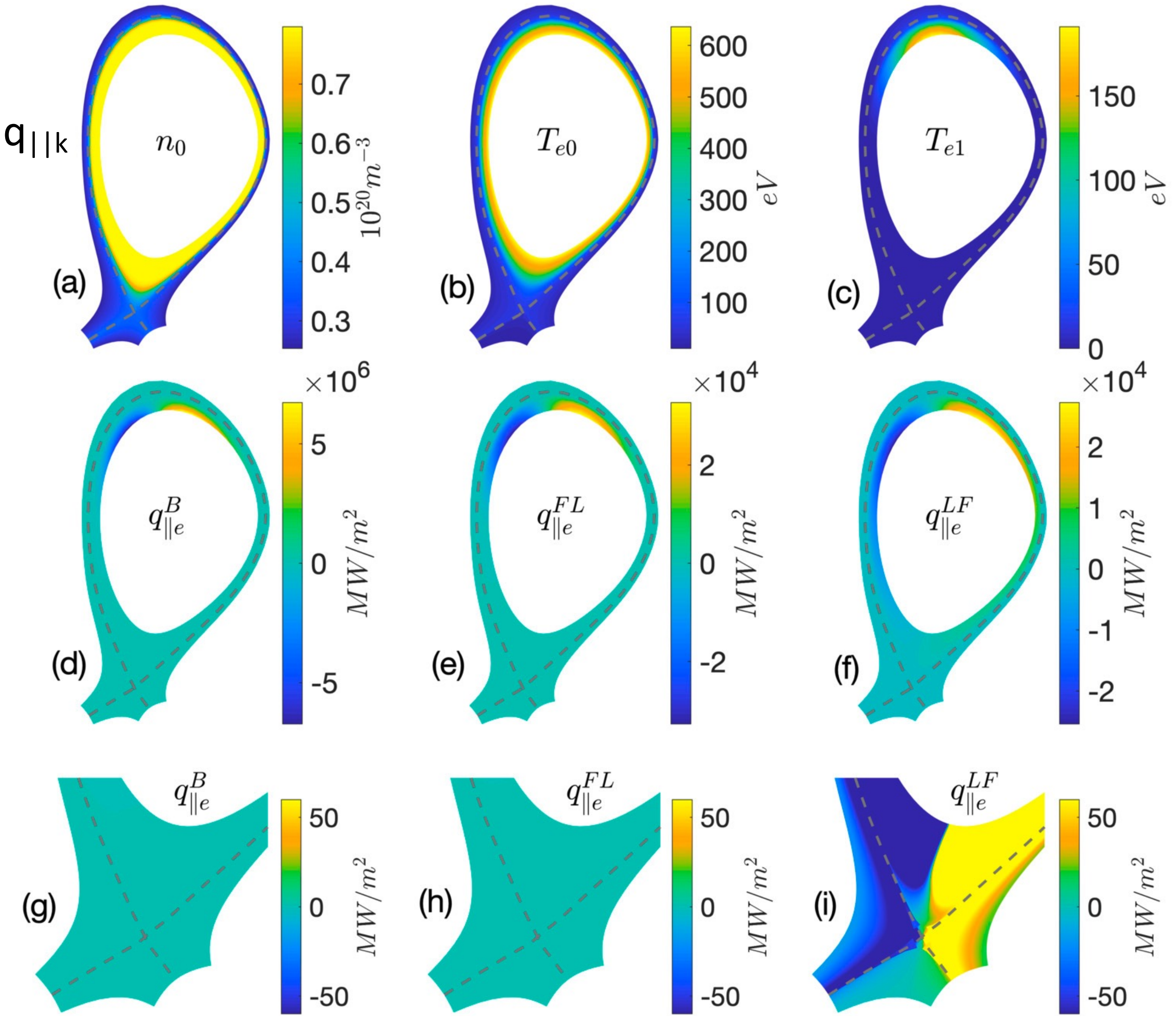


Drift reduced Landau fluid model for magnetized plasma turbulence simulations in BOUT++ framework

Ben Zhu et al, Computer Physics Communications, 267 (2021) 108079





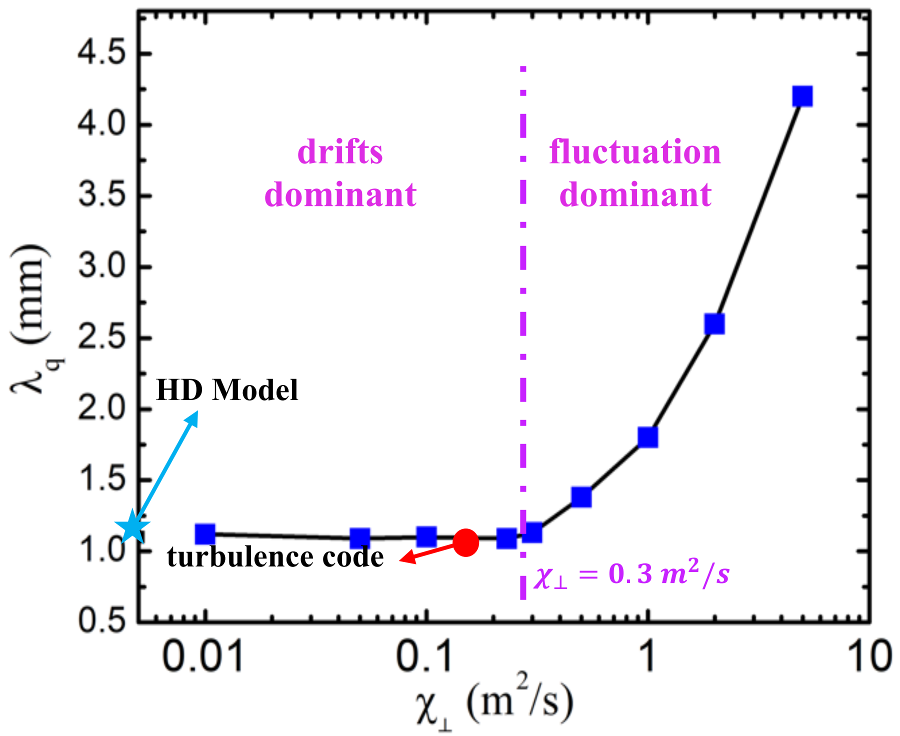


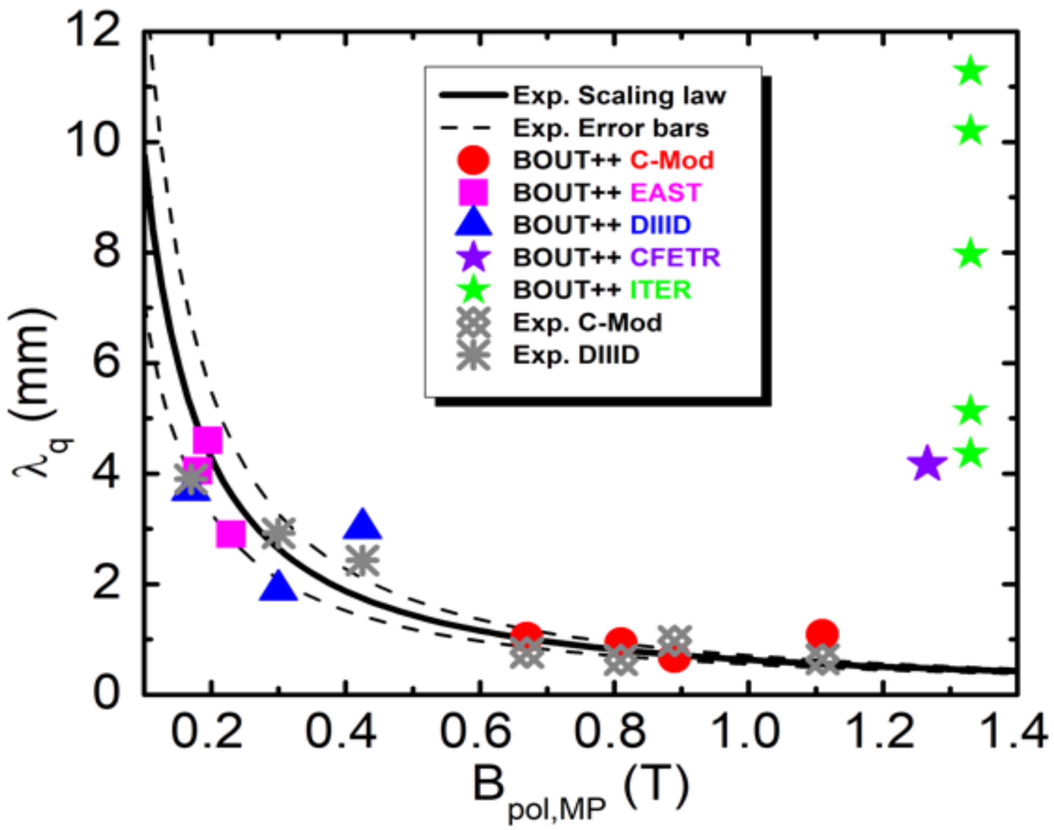
T_{e1} has a relatively large perturbation (30%) on the top portion of tokamak

- Braginskii model predicts $q_{\parallel}$ only at the tokamak top region where temperature gradient is finite (thus, "local" model) and its amplitude is about two orders of magnitude larger than either flux-limited or the Landau fluid estimate.
- The Landau fluid closure obviously exhibits the "nonlocal" effect as the predicted parallel heat flux extends to the region where local temperature gradient vanishes (e.g., the tokamak bottom region).
- only the Landau fluid closure is able to consistently enforce the ambipolar sheath heat flux boundary condition q_{sheath} at the divertor targets

BOUT++ simulations predict that the divertor heat flux width of ITER & CFETR baseline target is broadened by ELMs

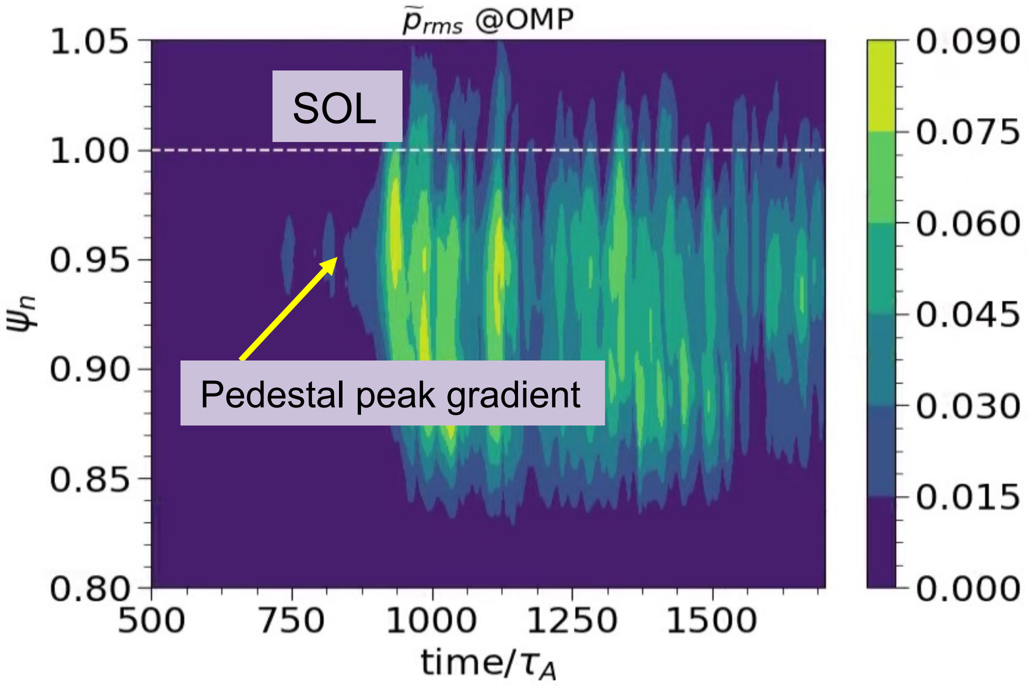
X.Q. Xu *et al* 2019 *Nucl. Fusion* **59** 126039

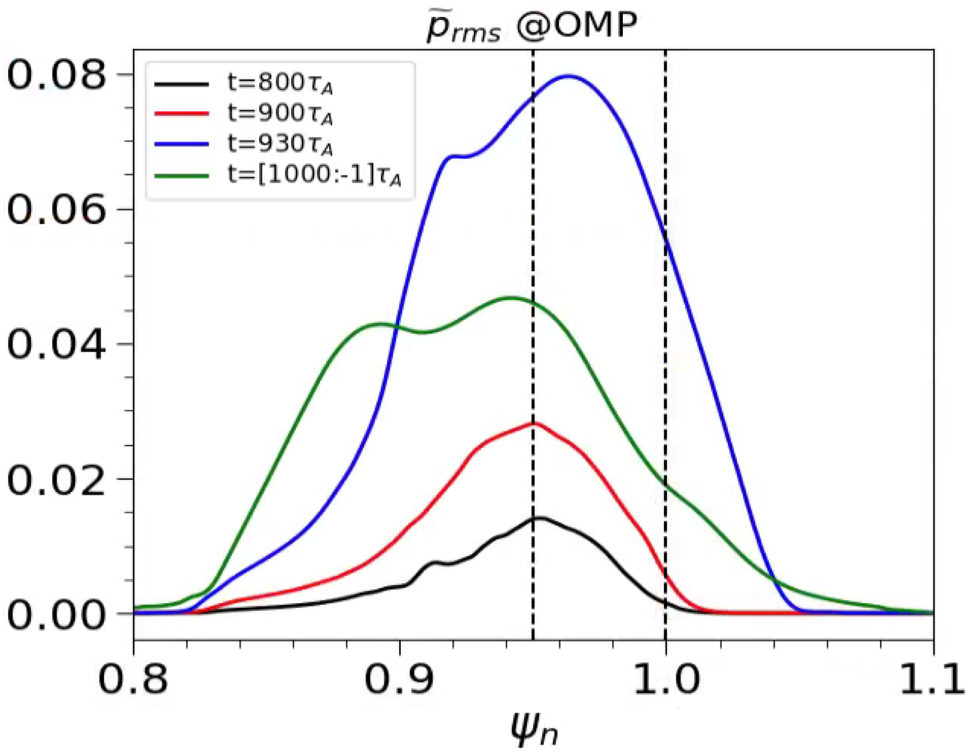




- When $\chi > \chi_{crit}$, radial transport transits from a drift to a fluctuation-dominated regime
  - Bohm diffusion typically yields $\chi^{\mathrm{Bohm}} \gg \chi_{crit}$
- The divertor heat flux width is correlated with change in pedestal height
- ITER & CFETR are in fluctuation dominant regime because the drifts are reduced due to their large size R

BOUT++ 6-field turbulence nonlinear simulations show that turbulence is generated inside pedestal & spread into the SOL

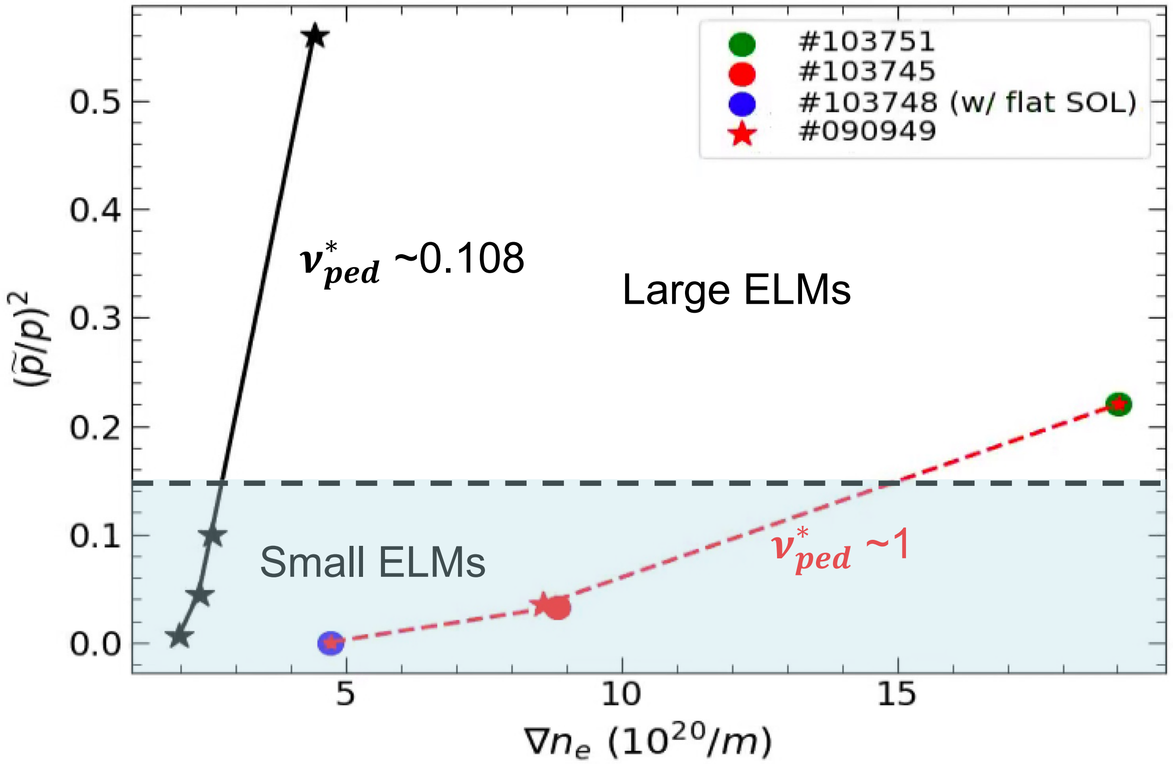


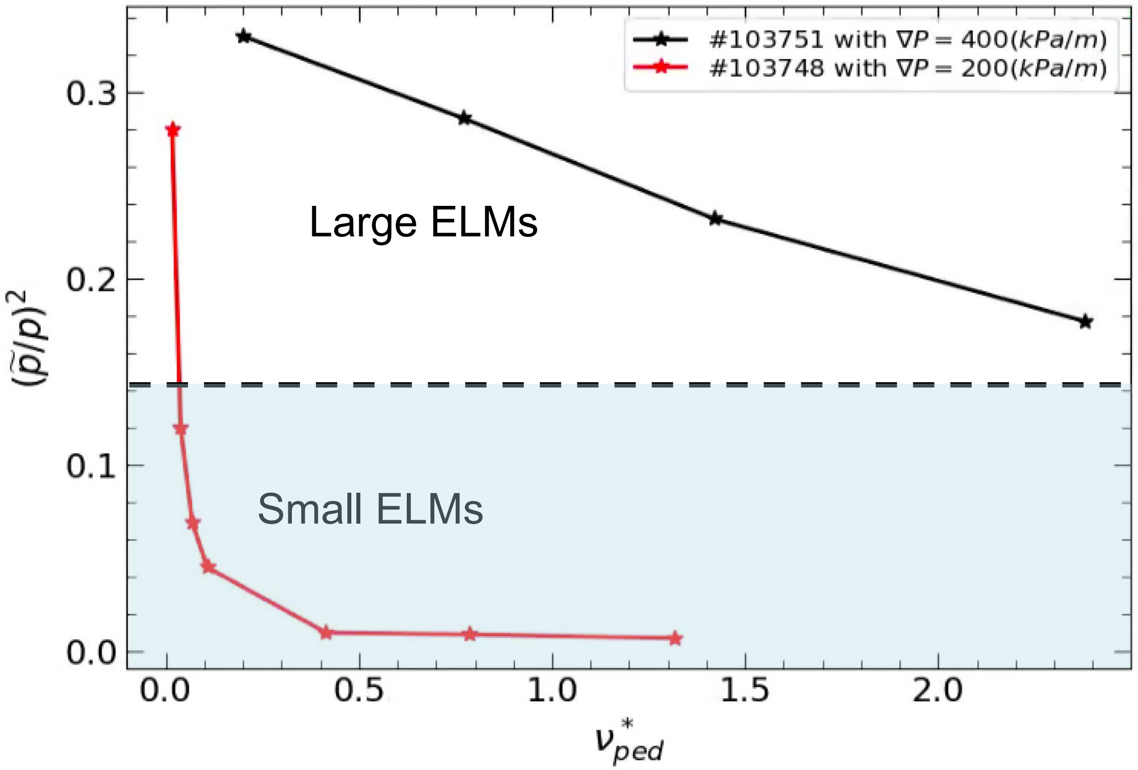


Nami Li et al 2022 Nucl. Fusion 62 096030

BOUT++ turbulence simulations show that turbulence spreading increases as pedestal density gradient increases and pedestal collisionality decreases

N. Li, UI01.00001 64th APD DPP





- Fluctuation intensity $(\tilde{p}/p)^2$ at LCFS increases as pedestal gradient (∇n_e or ∇P_0) increases
  - Small ELMs
    - ✓ With high ν^*_{ped}: wide range of ∇n_e or ∇P_0 window
    - ✓ With low ν^*_{ped}: narrow range of ∇n_e or ∇P_0 window

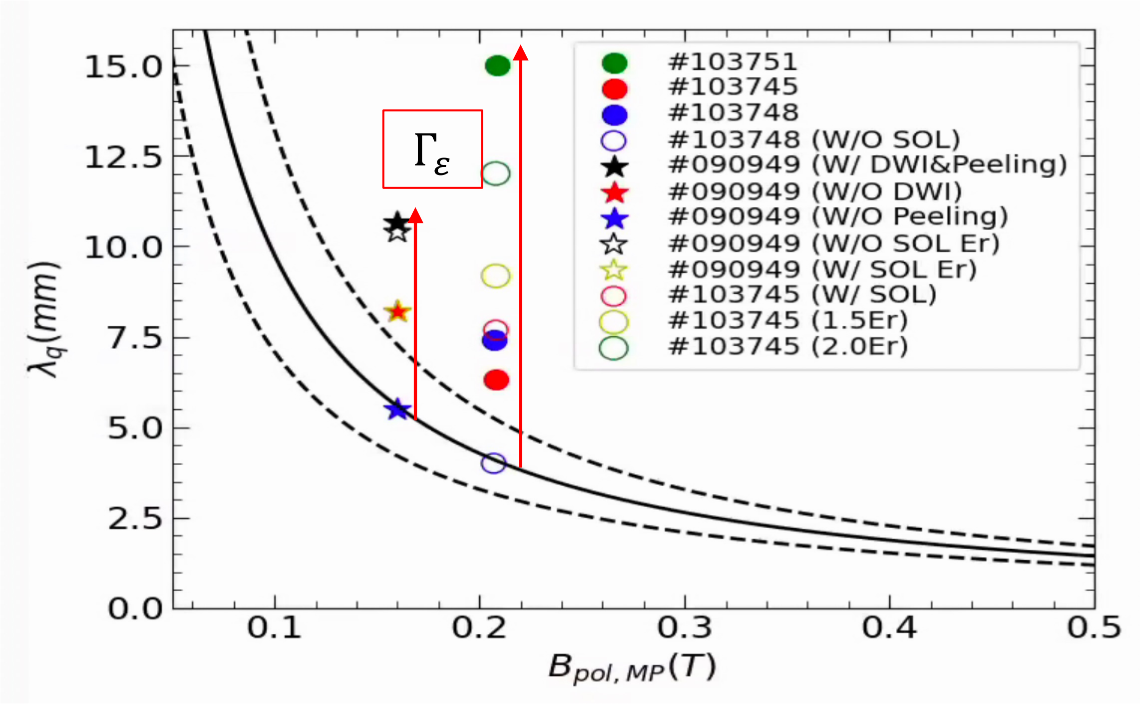
- Fluctuation intensity $(\tilde{p}/p)^2$ at LCFS increases as pedestal collisionaltiy ν^*_{ped} decreases
  - Small ELMs
    - ✓ With small ∇n_e: wide range of ν^*_{ped} window
    - ✓ With large ∇n_e: very high ν^*_{ped}

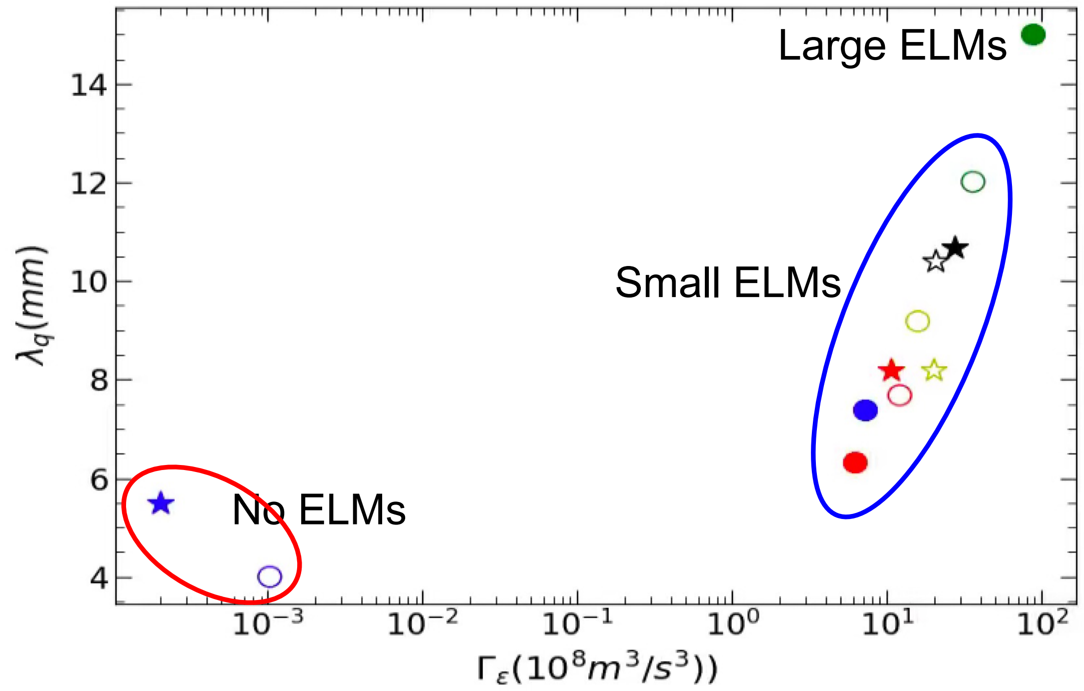
BOUT++ turbulence simulations show λq is significantly broadened from ELM-free to small ELM regime as fluctuation energy intensity flux increases

N. Li, UI01.00001 64th APD DPP

- **Divertor heat flux width is broadened by a larger radial turbulence transport**
  - ✓ **Fluctuation energy intensity flux Γ_ε at LCFS measures the turbulence spreading from pedestal into the SOL**
  - ✓ **Heat flux width increases with Γ_ε increasing**

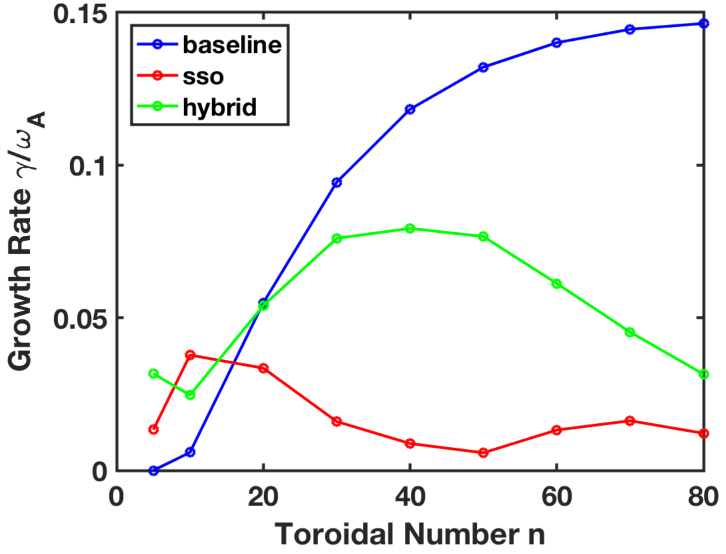
$$\Gamma_\varepsilon = c_s^2\langle \tilde{V}_r (\tilde{p}/p)^2 \rangle$$

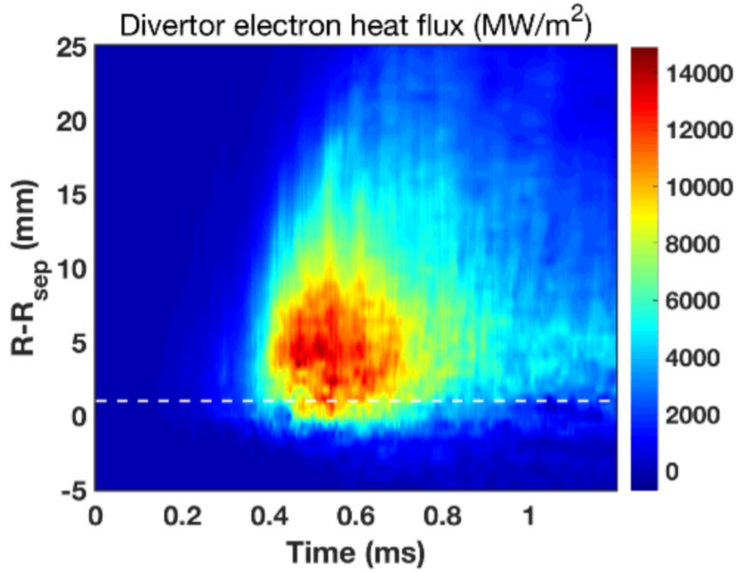




BOUT++ simulations of divertor heat load for ITER scenarios

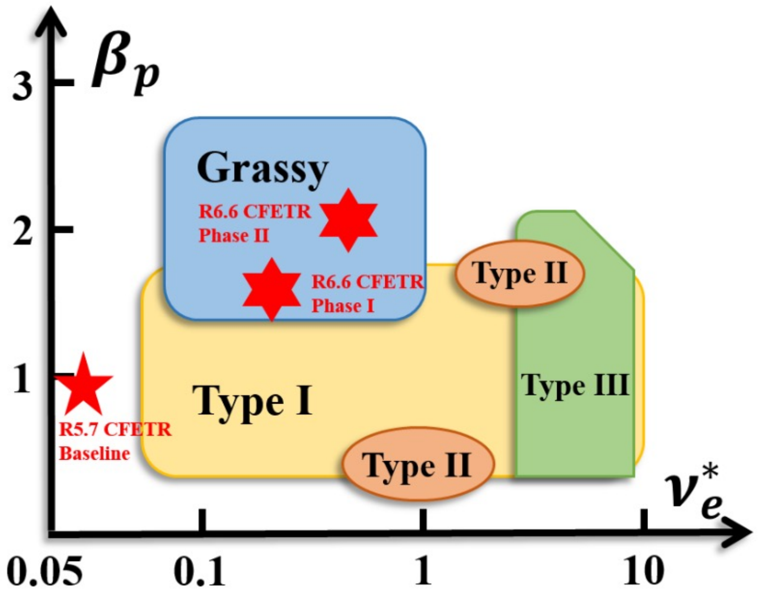
Xueyun Wang et al 2022 Nucl. Fusion 62 026024

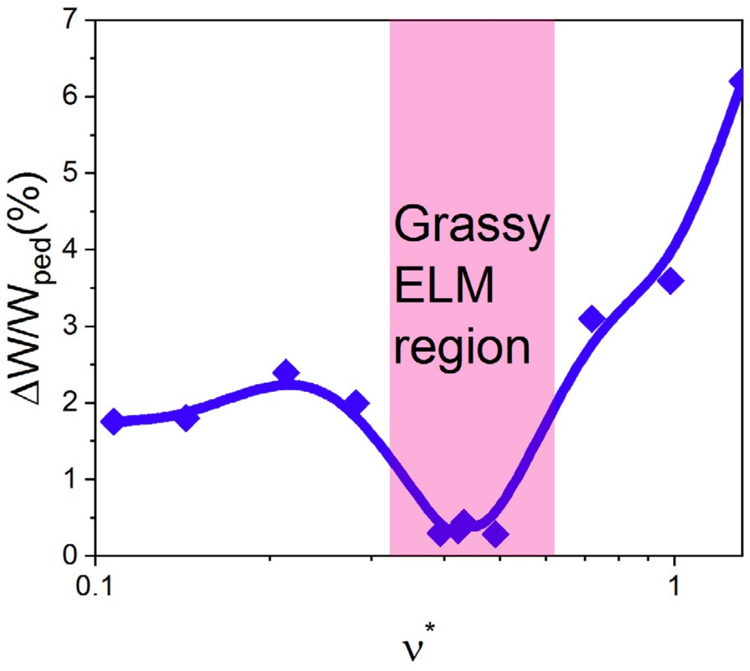


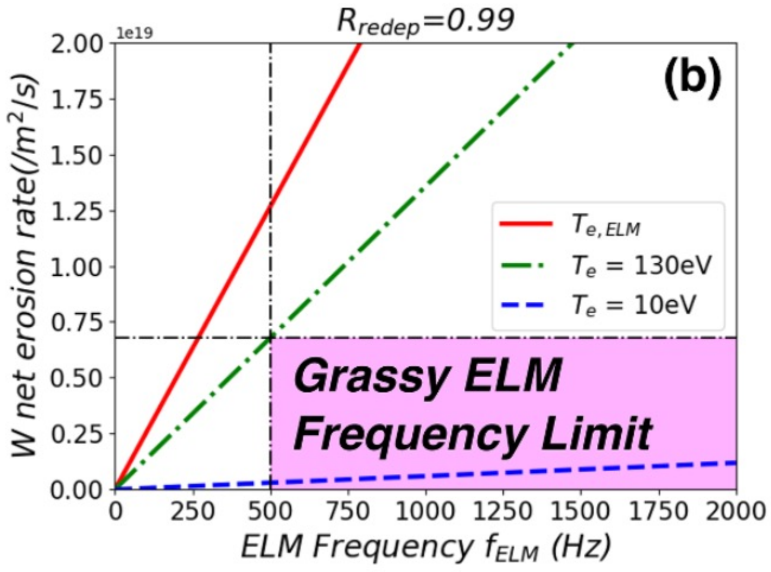


scenarios	baseline	hybrid	SSO
λ_q^u (mm)	11.28	10.76	9.85
B_p/B_t	~0.1	~0.08	~0.06
f_x	2.95	3.45	4.66
R_t	6.2	6.2	6.35
I_p(MA)	15	11.5	10
P_{ped}(kPa)	150	100	100
W(MJ)	189	126	126
ε_{target} limit	0.16	0.2	0.22
ΔW/W limit $\alpha_{div} = 90°$	0.2%	0.5%	0.6%
ΔW/W limit $\alpha_{div} = 30°$	0.4%	1.0%	1.2%

CFETR edge and boundary design are benefited from BOUT++ modeling







- CFETR: China Fusion Engineering Test Reactor
- ELM characteristic prediction for CFETR different design phases[1,3,4]
- Divertor heat flux width and divertor heat load are estimated for divertor engineering design[2,5]
- The idea of an operation with grassy ELMs is adopted by the CFETR Design Group
  - Compatibility of high core performance and tolerable divertor load

[1] Zeyu Li et al. NF 2018
[2] X. Q. Xu et al., NF 2019
[3] Y. R. Zhu et al. NF 2020
[4] T. F. Tang et al., NF 2021
[5] Zeyu Li et al. PPCF 2021

Small ELMs with quasi-continuous exhaust is a promising regime for a tokamak fusion power Plant

- **Good energy confinement**
- **Comparable with inter-ELM level of divertor heat flux**
- **Broadening divertor heat flux**
- **Quasi-continuous particle and power exhaust to divertors**
- **Divertor plasma detachment is required for low divertor Te to maintain acceptable tungsten erosion**