Latest developments in BOUT++ boundary plasma turbulent transport simulations

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

Xueqiao Xu
In collaboration with BOUT++ team
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-06: code refactoring using differential operator approach, high order FD, verification

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

- Xu, Umansky, Dudson & Snyder, CiCP, V. 4, 949-979 (2008).
- Xu, Dudson, Snyder et al., PRL 105, 175005 (2010).

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

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

2000 2005 2009 2023

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

https://bout.llnl.gov
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BOUT++ have been products of broad international collaborations
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
  
  [Images of various scientific figures and data]

Walkden, et al. 2022, COMMUNICATIONS PHYSICS

https://bout.llnl.gov/publications
http://boutproject.github.io/publications/
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 ISTTK: a multi-code fluid validation

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

- Undertaken through the framework of EUROfusion Enabling Research
- ISTTK 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 $l_{sat}$ fluctuation
3D STORM turbulence simulations of the MAST and comparison with experimental measurements

- 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 $T_e$ perturbation

• The agreement between experiment and simulation is robust to changes in the initial $T_e$ 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


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 $\psi_N=1.008$
**Drift reduced Landau fluid model for magnetized plasma turbulence simulations in BOUT++ framework**

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

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

- Braginskii model predicts \( q_1 \) 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 \( q_{\text{sheath}} \) at the divertor targets

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- **Diagram Description**
  - *Left Panel*
    - Plot showing \( k_{||}/\lambda_{mfp} \) vs. \( \hat{\nu}_{||}/(m \omega_{ci} \bar{v}_{||}) \).
    - Includes collisionless and collisional limits.
  - *Right Panel*
    - Graphs showing temperature, density, and heat flux profiles for different models.
    - \( q_{||} \), \( n_{0} \), \( T_{e0} \), \( T_{e1} \), \( q_{Lc}^{B} \), \( q_{Lc}^{F} \), etc.
    - Colored regions indicate magnitude and direction of heat flux, with color bars for MW/m².
BOUT++ simulations predict that the divertor heat flux width of ITER & CFETR baseline target is broadened by ELMs

- When $\chi > \chi_{\text{crit}}$, radial transport transits from a drift to a fluctuation-dominated regime
  - Bohm diffusion typically yields $\chi^\text{Bohm} \gg \chi_{\text{crit}}$
- 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 $R$

X.Q. Xu et al 2019 Nucl. Fusion 59 126039
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 \((\bar{p}/p)^2\) at LCFS increases as pedestal gradient \((\nabla n_e \text{ or } \nabla P_0)\) increases
  - Small ELMs
    - With high \(v_{ped}^*\): wide range of \(\nabla n_e \text{ or } \nabla P_0\) window
    - With low \(v_{ped}^*\): narrow range of \(\nabla n_e \text{ or } \nabla P_0\) window

- Fluctuation intensity \((\bar{p}/p)^2\) at LCFS increases as pedestal collisionality \(v_{ped}^*\) decreases
  - Small ELMs
    - With small \(\nabla n_e\): wide range of \(v_{ped}^*\) window
    - With large \(\nabla n_e\): very high \(v_{ped}^*\)
BOUT++ turbulence simulations show $\lambda q$ 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 $\Gamma_\varepsilon$ at LCFS measures the turbulence spreading from pedestal into the SOL
  - Heat flux width increases with $\Gamma_\varepsilon$ 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

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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