SciDAC ISEP:

Integrated Simulation of Energetic Particles in Burning Plamsas

Principal Investigator:

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Ronald Waltz, General Atomics (GA)
Robert Falgout, Lawrence Livermore National Laboratory (LLNL)
Scott Klasky, ORNL
William Tang, PPPL
Samuel Williams, Lawrence Berkeley National Laboratory (LBNL)

ISEP motivation

- Confinement of energetic particles (EP) is a critical issue for burning plasmas since ignition in ITER relies on self-heating by energetic fusion products (α-particles)
- Plasma confinement properties in *new* ignition regime of self-heating by α-particles is one of the most uncertain issues in ITER/FPP (Fusion Pilot Plant)
- **EP turbulence and transport**: EP excite meso-scale instabilities and drive large transport, which can degrade overall plasma confinement and threaten machine integrity
- **Interaction between EP and thermal plasmas**: EP can strongly influence microturbulence responsible for turbulent transport of thermal plasmas and macroscopic magnetohydrodynamic (MHD) instabilities potentially leading to disruptions
- SciDAC ISEP: integrated simulations of EP turbulence by treating relevant physical processes from micro to macro scales on same footing

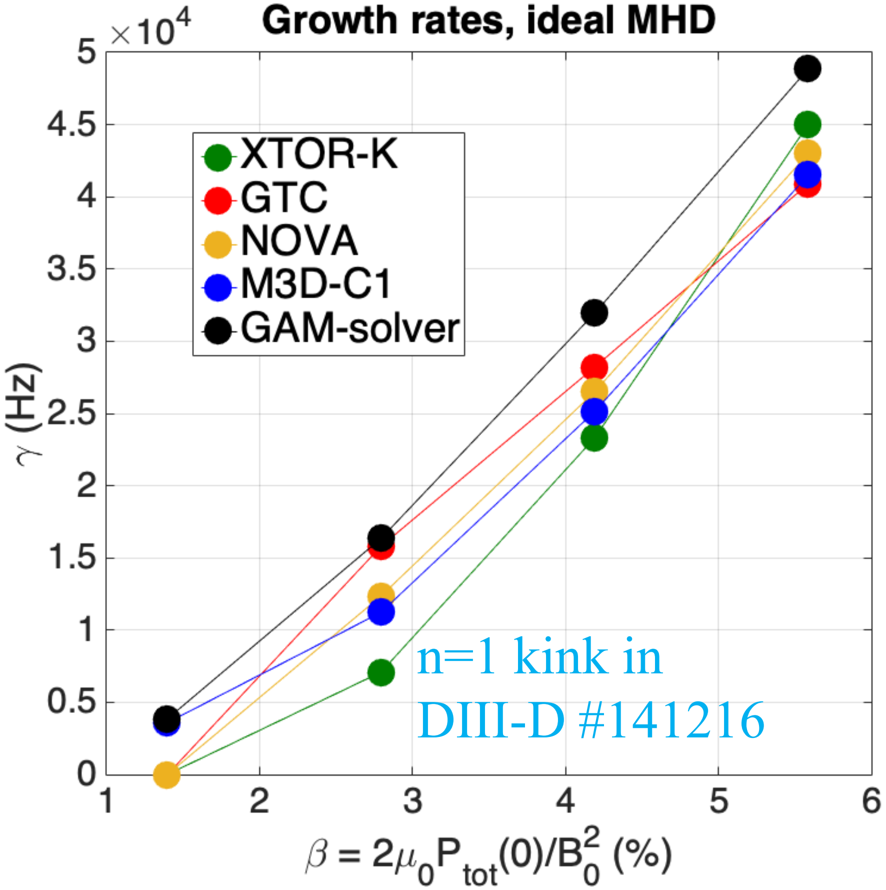
  → Develop EP module in WDM (whole device modeling) for ITER/FPP design & operation

ISEP overview

- Developed integrated simulation of EP physics using gyrokinetic codes GTC & GYRO, and kinetic-MHD codes FAR3D & M3D-C1
  - → EP physics needed for developing reduced EP transport models & for extrapolating to ITER/FPP
  - → Cross-scale simulations at exascale requires computational partnership
- Developed a hierarchy of complementary EP transport models, and provided EP modules in TRANSP & Atom2 for WDM
  - → Reduced models: physics based CGM & RBQ, interpretive Kick, deep learning FRNN
  - → First-principles ISEP framework (based on GTC)
  - → Verification & validation (V&V)
- OFES/ASCR computational partnership
  - → Workflow/data management
  - → Solvers
  - → Optimization & portability

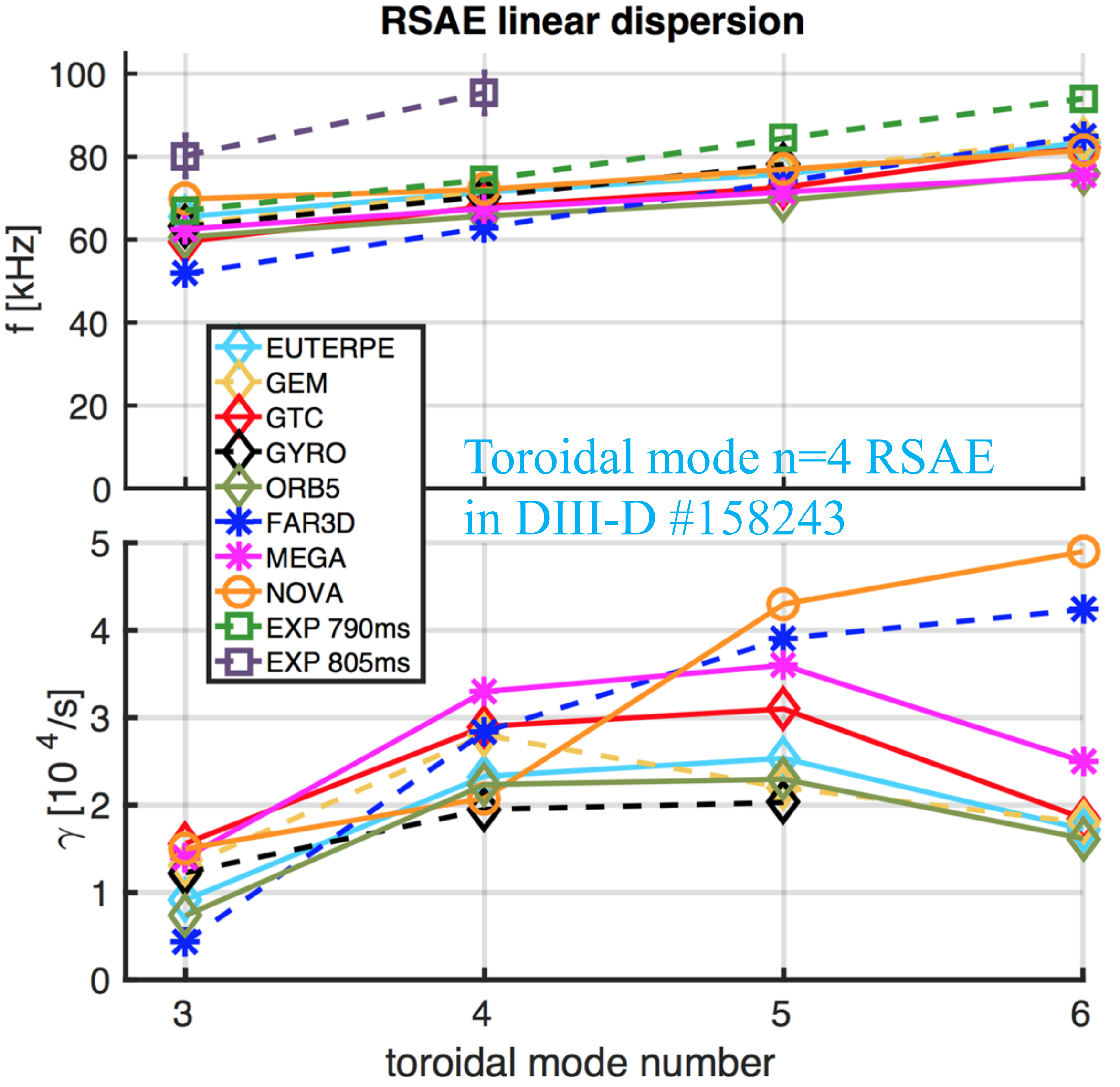
Accomplishments: V&V for ISEP framework using DIII-D data

- Largest V&V for linear Alfven eigenmode (AE)
- First V&V for gyrokinetic simulation of MHD modes (kink, fishbone)



n=1 kink in DIII-D #141216

Brochard, submitted to NF (2021)

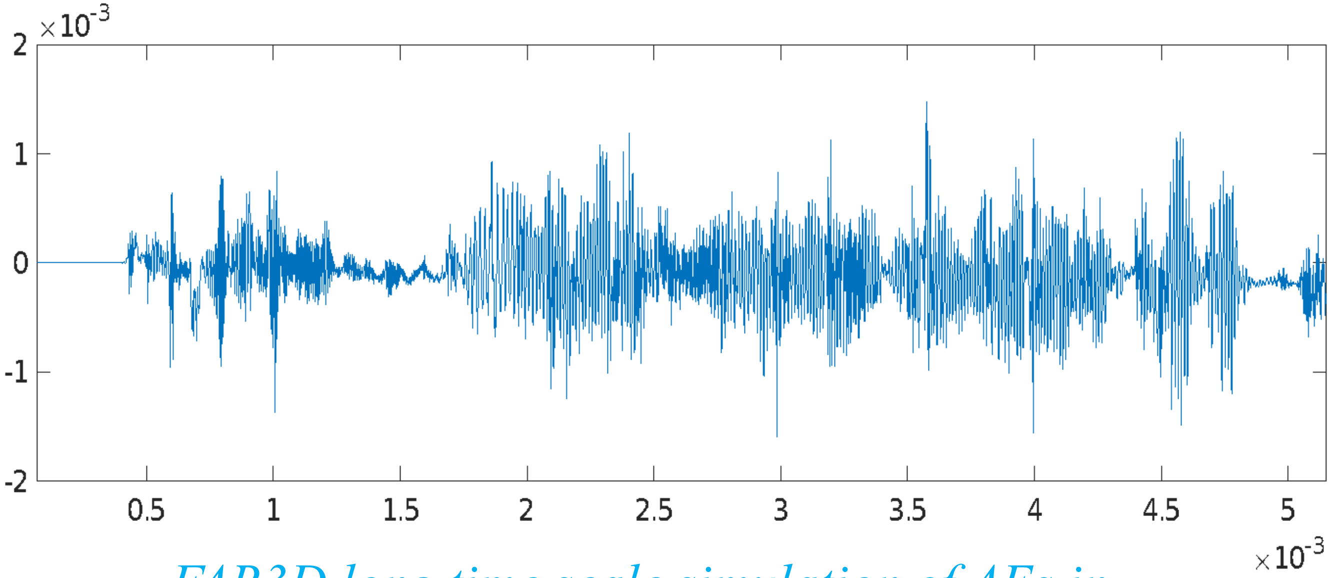


Toroidal mode n=4 RSAE in DIII-D #158243

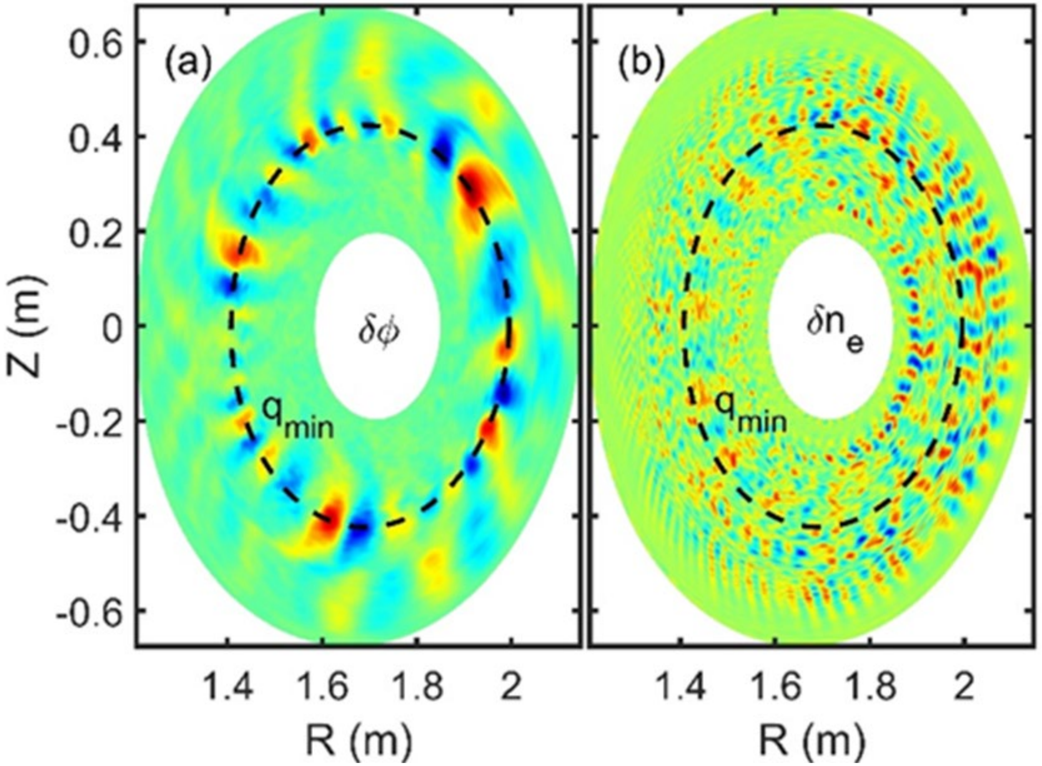
Taimourzadeh, NF59, 066006 (2019)

Accomplishments: integrated simulation of EP turbulence

- EP integrated simulation enabled by computational partnership
  - → Largest cross-scale gyrokinetic simulations find AE regulated by microturbulence, AE amplitude & EP transport agree well, for the first time, with experimental measurements. Physics incorporated in RBQ
  - → Kinetic-MHD long-time scale AE simulations show similar frequency spectrum and amplitude variation as observed in experiments
- Presentation by Spong



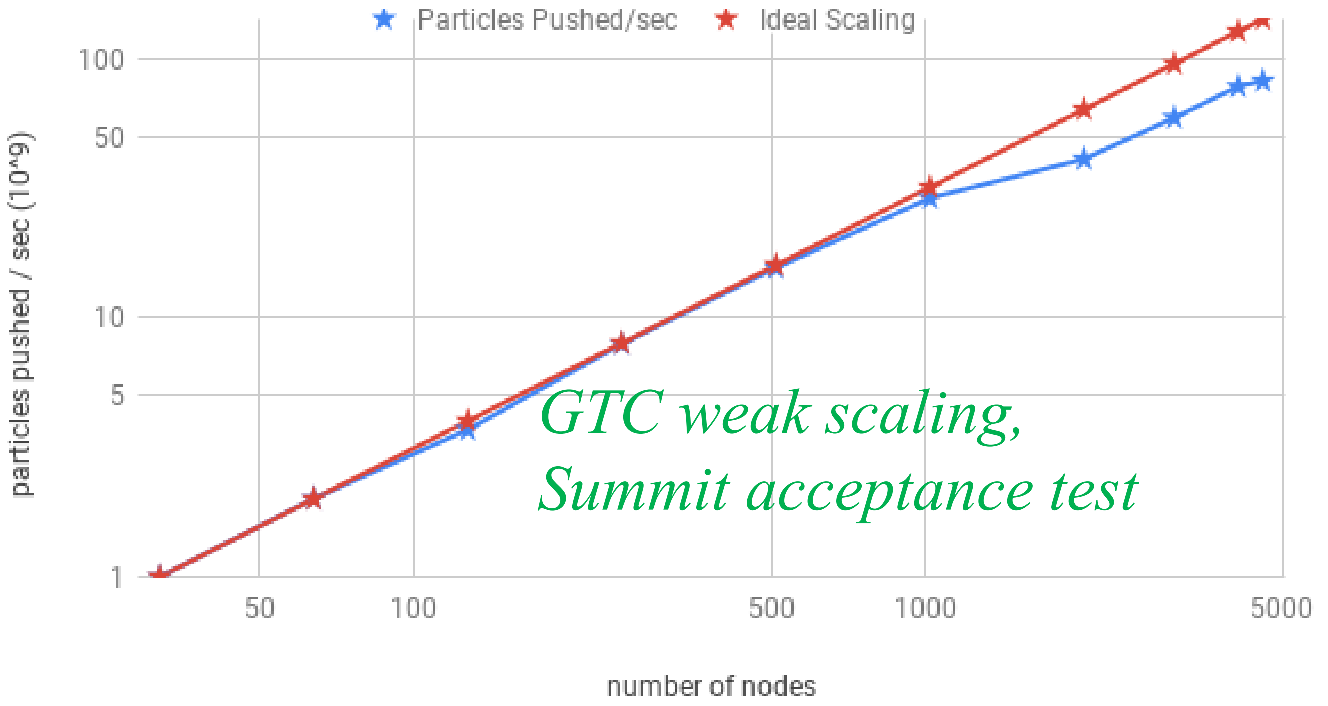
FAR3D long time scale simulation of AEs in DIII-D #176523, Spong, NF61, 116061(2021)



GTC simulation of RSAE-microturbulence in DIII-D #159243, Liu, submitted to PRL (2021)

Computational partnership: collaboration & benefit

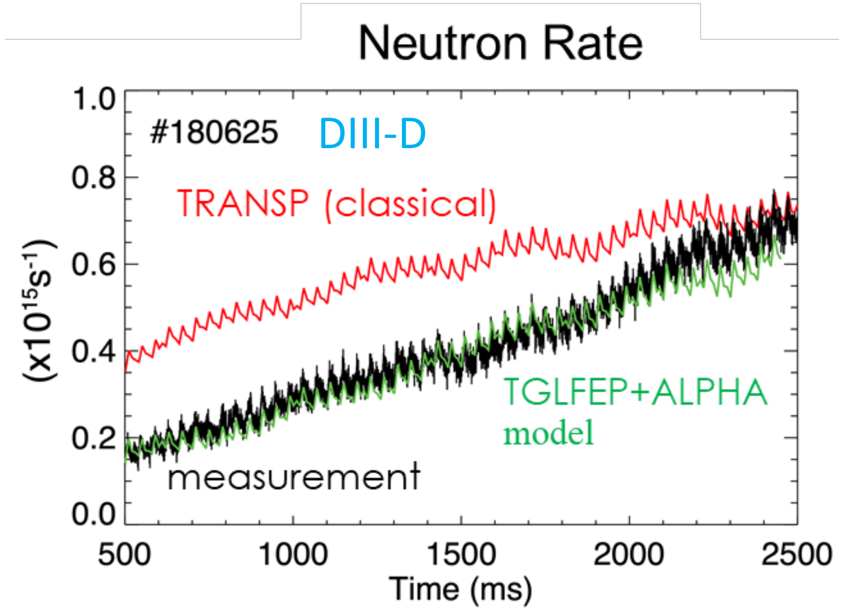
- Optimized I/O to reduce overhead when running at scale; GTC was "first full" application on Summit to get over 2 TB/s [Wan, ICCM2019 invited talk]
- Optimized hypre on GPU leads to GTC Poisson solver 3X speedup on Summit
- Optimized GTC scales up to whole machine in Summit [Zhang, WACCPD 2018 Workshop at SC18]
- 5th year: optimizations for Perlmutter & Frontier, further development of FRNN/SGTC, workflows & I/O
- No-cost collaborations:
  → ASCR CAAR
  → NVIDIA, AMD
  → Google, Microsoft
  → RAPIDS, FASTMath
- Presentation by Williams

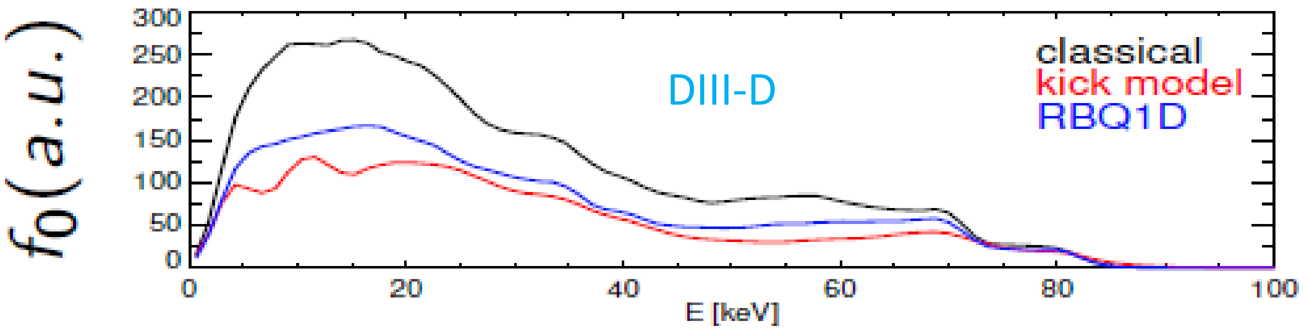


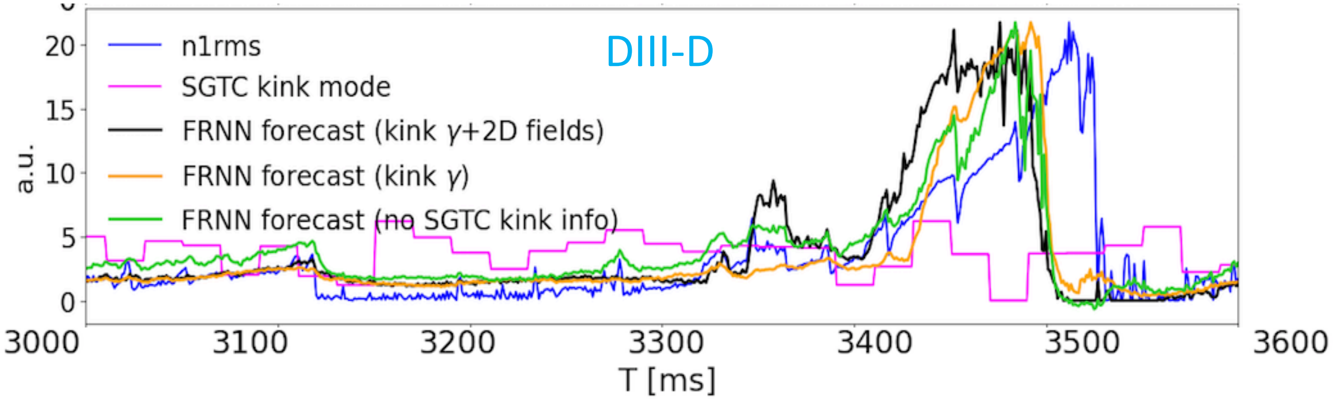
GTC weak scaling, Summit acceptance test

Accomplishments: EP modules with predictive capability

- Verification of fast ion distribution calculated by RBQ and Kick models [Duarte, APS-DPP2020 invited]
- CGM diffusion coefficient added to TRANSP for neutron prediction in agreement with experiments [Bass, IAEA2018 oral; Collins, IAEA2021 oral]
- Improved FRNN disruption prediction by adding NTM physics (n=1 signal, NTM drive, surrogate model SGTC trained by GTC simulations of 5000+ DIII-D experiments) [Tang, IAEA2021 oral; Dong, J. Machine Learning for Modeling & Computing 2, 49 (2021)]
- Presentation by Waltz & Gorelenkov







Plan for 5th year

- OFES FY22 TPT & ITPA: Energetic particle confinement properties of ITER operation scenarios will be comprehensively assessed using global gyrokinetic codes, hybrid MHD codes, and reduced EP transport models
  - → largest ITER simulations using 15 codes (9 US + 4 EU + 2 Asia)
- Further develop EP modules for WDM
- Perform gyrokinetic full-f long time AE simulation
- Perform integrated simulation of MHD, AE, and microturbulence

	Microturbulence	AE	MHD: kink, fishbone, sawtooth
Gyrokinetic	GTC, GYRO	GTC, GYRO, LIGKA, ORB5	GTC
Kinetic-MHD		FAR3D, GAM-solver, HYMAGYC, M3D-C1, MEGA, NOVA-K	FAR3D, GAM-solver, HYMAGYC, M3D-C1, MEGA, NOVA-K, XTOR-K
Reduced model		CGM, KICK, RBQ	KICK, FRNN

Looking ahead: most critical but still unsolved problems

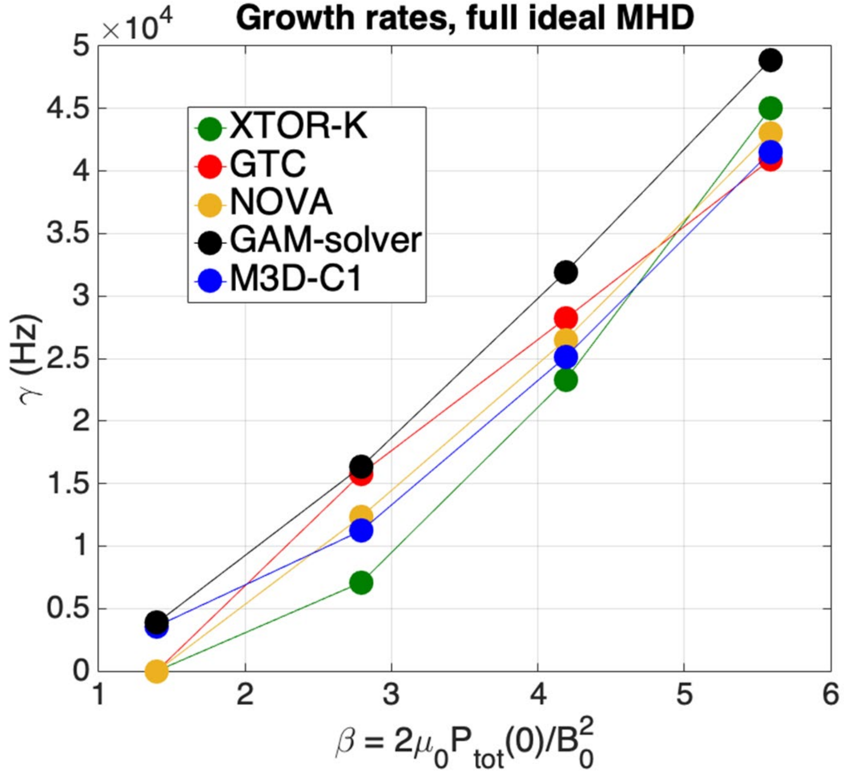
- Multi-physics, cross-scale coupling in EP transport, extrapolation to ITER/FPP
- Physics-based, validated EP transport module in WDM for ITER/FPP design & operation
- Convergence of deep learning and model simulation, real time prediction & control
- Impacts on future OFES/ASCR partnership
  - → Data management
  - → New architecture, exascale
  - → Convergence between DL & model simulation
- Project impacts
  - → Paradigm shift to integrated gyrokinetic simulations of EP turbulence
  - → First reduced models for EP transport, first EP modules for WDM
  - → Simulated DIII-D, NSTX-U, ITER, JET, JT-60, EAST, HL-2A, KSTAR, LHD, W7-X, TJ-II, C2-W, …
  - → 115 Publications, 45 Invited talk
  - → 14 postdocs, 8 Students
  - → Bi-weekly ISEP meeting (~40 attendees, many from EU & Asia)

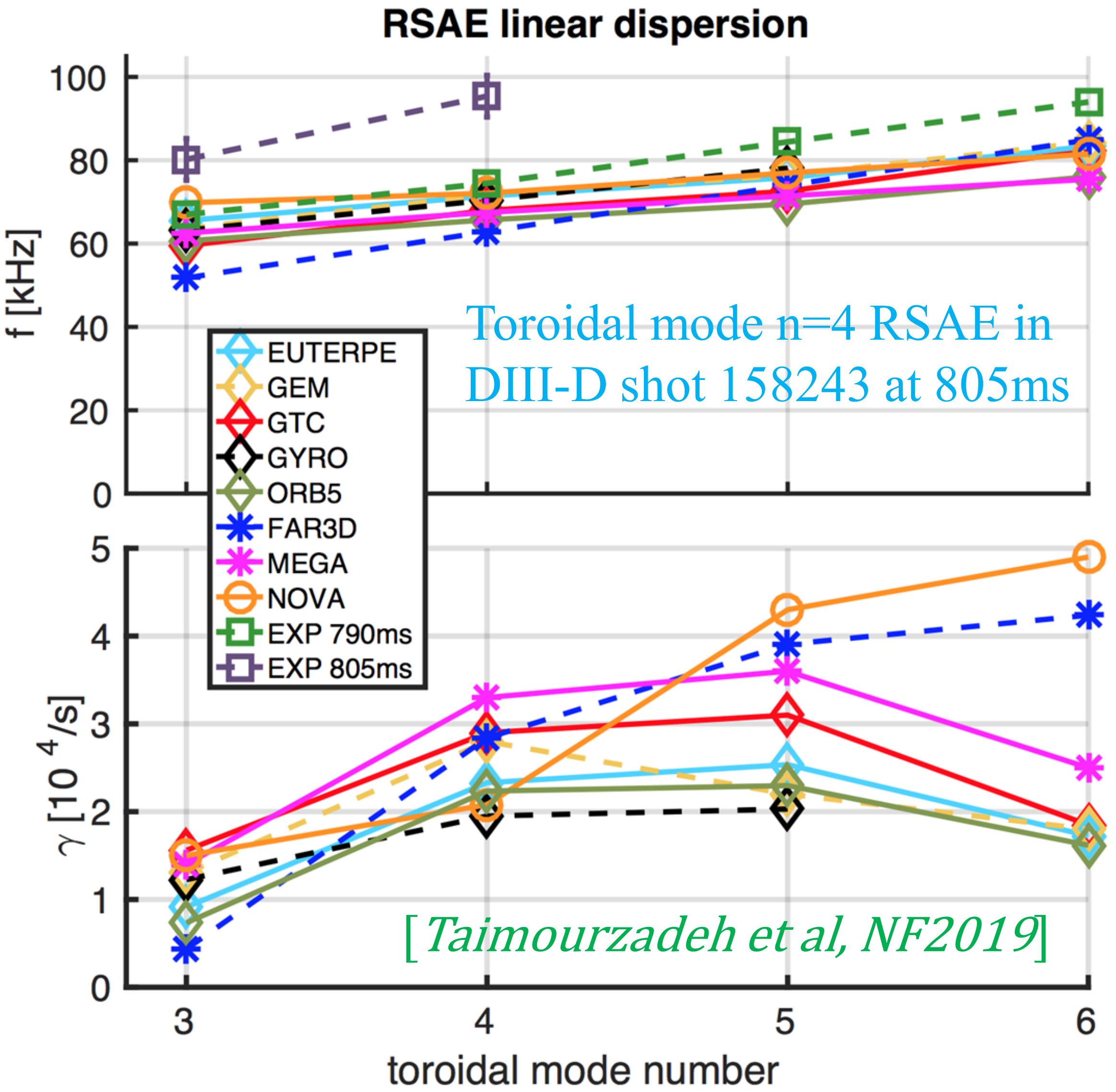
The ISEP center has emphasized development of energetic particle physics tools in preparation for integrated simulation/whole device modeling

- The ISEP members have contributed a suite of closely interrelated EP simulation models
  - Gyrokinetics (GTC, GYRO)
  - Hybrid models (M3D-C1)
  - Gyro-Landau closure (FAR3d)
- The diverse characteristics of these models have allowed us to address a range of different EP physics problems
- Collaboration with ASCR partners has led to significantly improved computational efficiencies

We regularly carry out multi-code V&V checks for DIII-D cases to check models and stimulate new development

- Linear Alfven eigenmode (AE) V&V completed
- Kink benchmark completed
- Fishbone benchmark ongoing
- SGTC module in FRNN



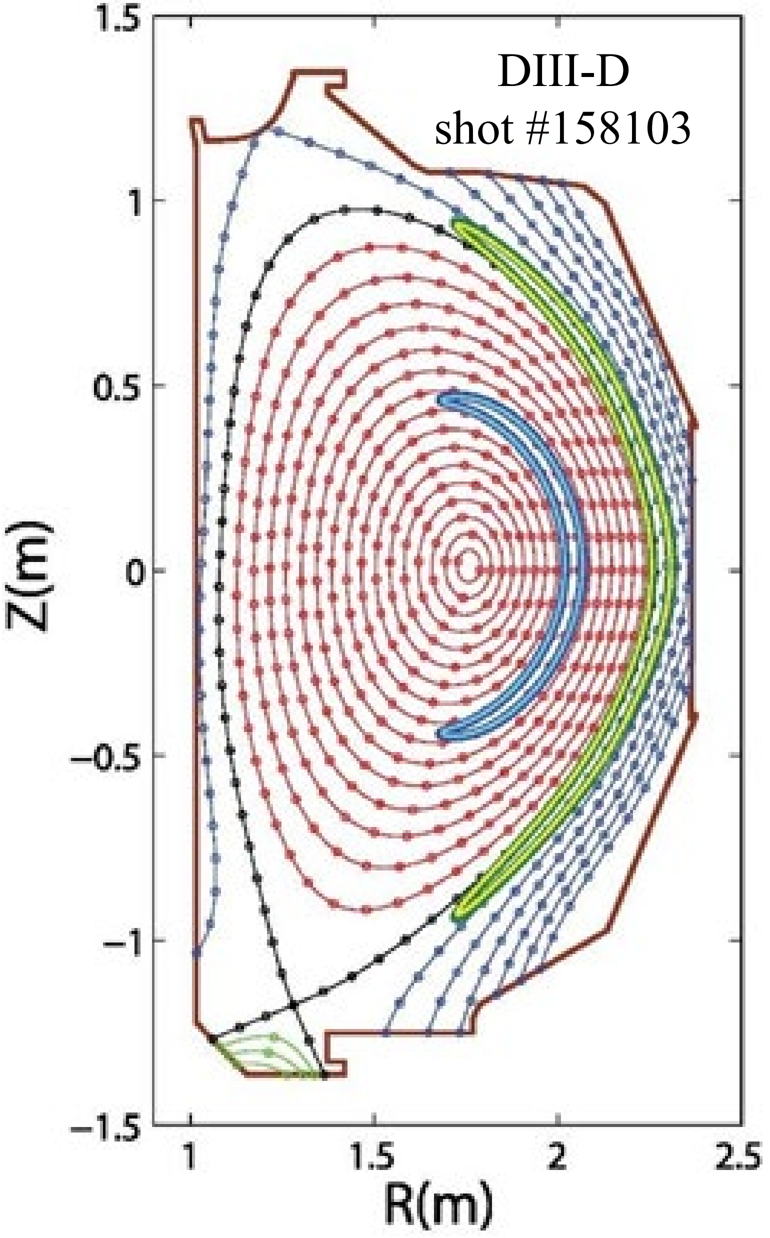


Toroidal mode n=4 RSAE in DIII-D shot 158243 at 805ms

[*Taimourzadeh et al, NF2019*]

The ISEP project provides a framework for first-principles integrated simulation

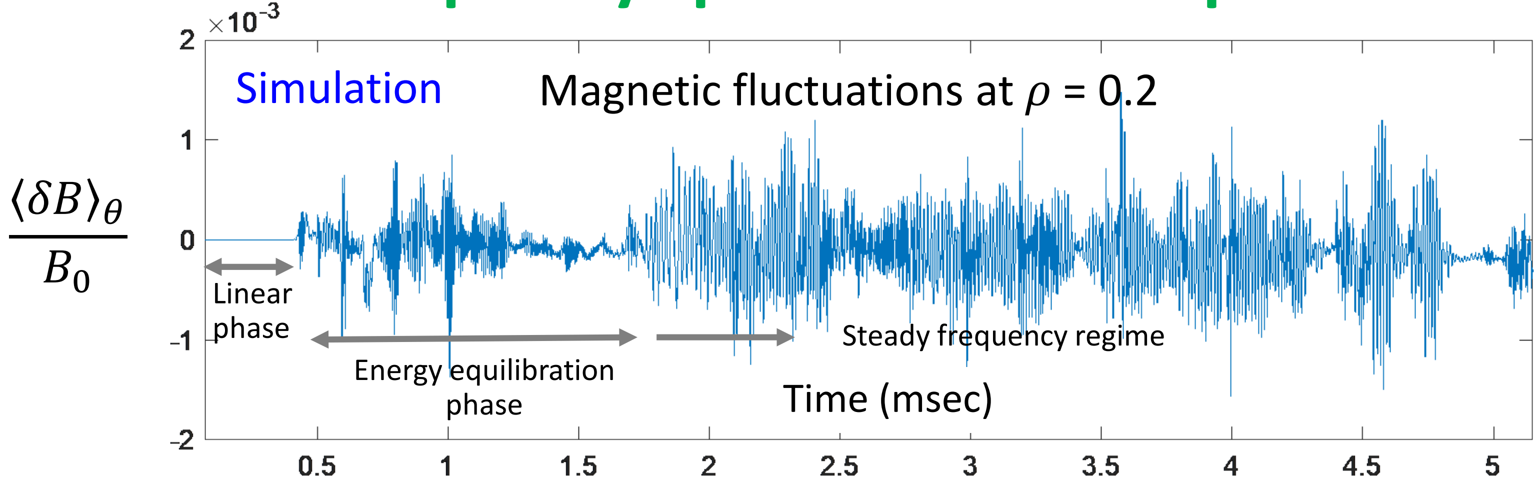
- ISEP framework based on gyrokinetic toroidal code GTC:
  - ✓ SciDAC GPS (01-11), GSEP (08-17), ISEP (17-21)
- First-principles, global, integrated simulation capability for nonlinear interactions of multiple kinetic-MHD processes
- Current capabilities
  - ✓ Global 3D toroidal geometry for tokamak, stellarator, FRC
  - ✓ Microturbulence: 5D gyrokinetic ions & electrons, electromagnetic compressible fluctuations, collisionless/collisional tearing modes
  - ✓ MHD and energetic particle (EP): Alfven eigenmodes, kink, resistive tearing modes
  - ✓ Neoclassical transport: Fokker-Planck collision operators
  - ✓ Radio frequency (RF) waves: 6D Vlasov ions
- Large user community (>40 users/developers); Broad impacts to fusion (12 papers in PRL, Science, Nature Comm.)

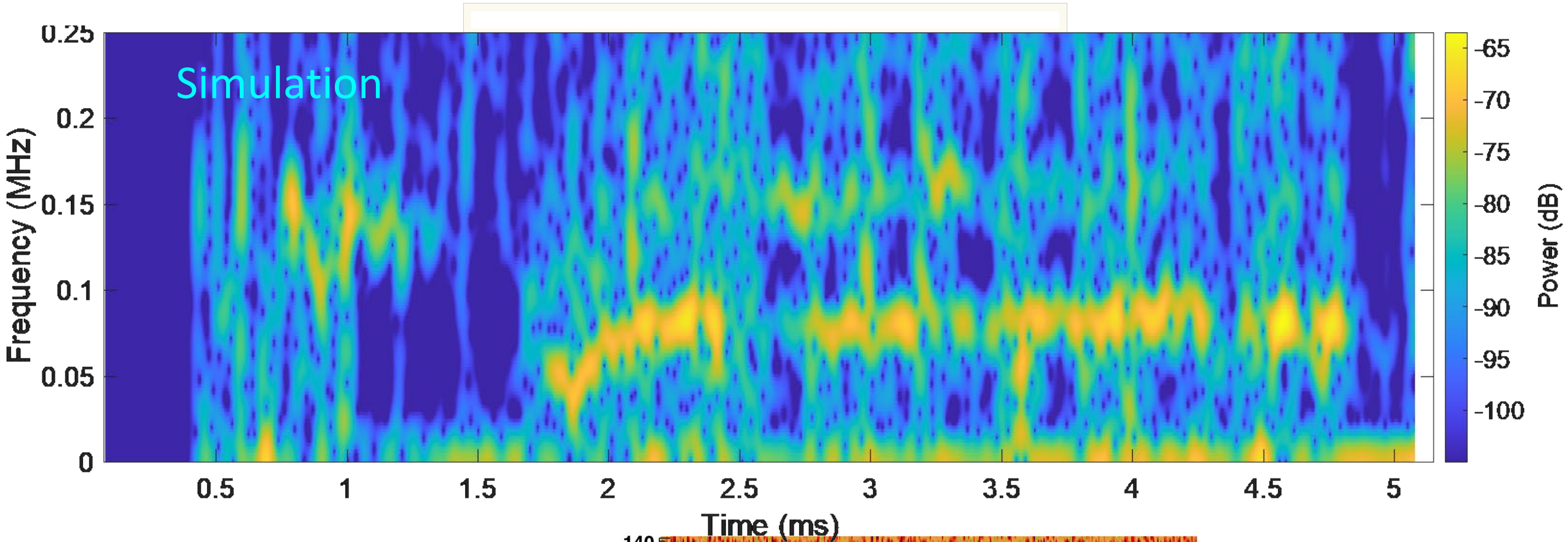


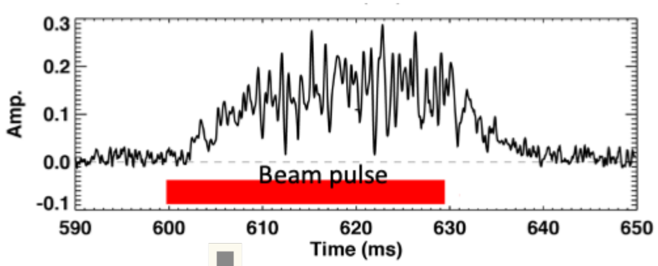
Z. Lin et al, Science 281, 1835 (1998)

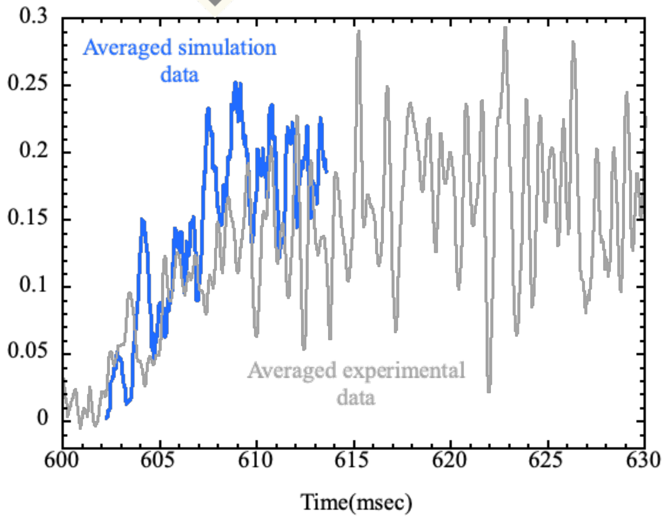
Open source: sun.ps.uci.edu/GTC

Long-time scale FAR3d nonlinear simulations of pulsed DIII-D Alfvén instability show similar frequency spectrum and amplitude variation as experiment

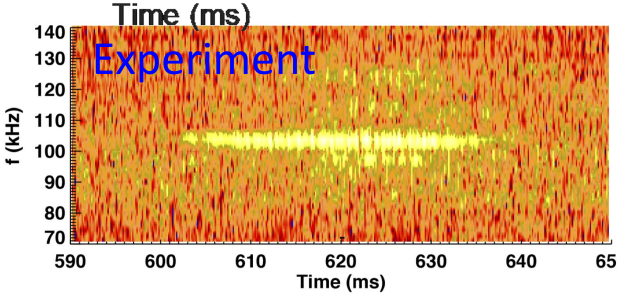






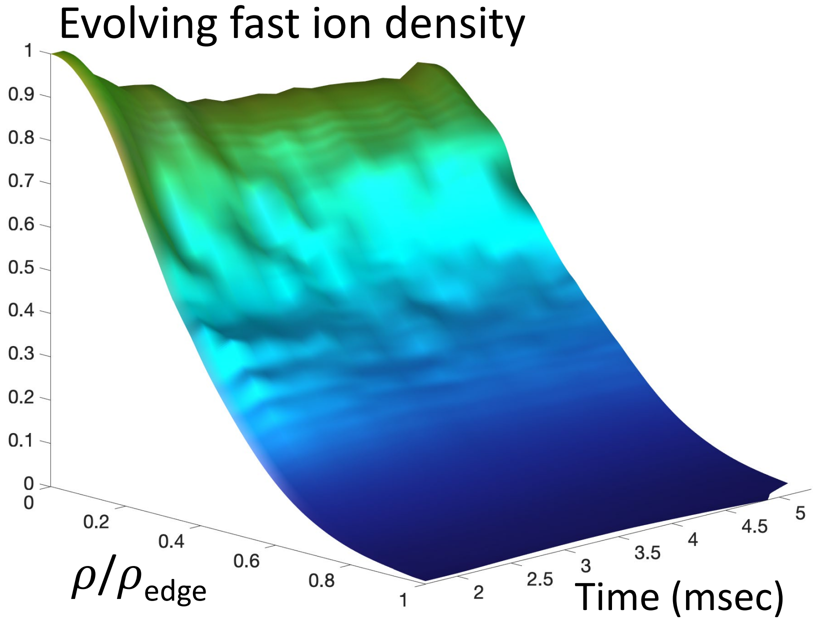


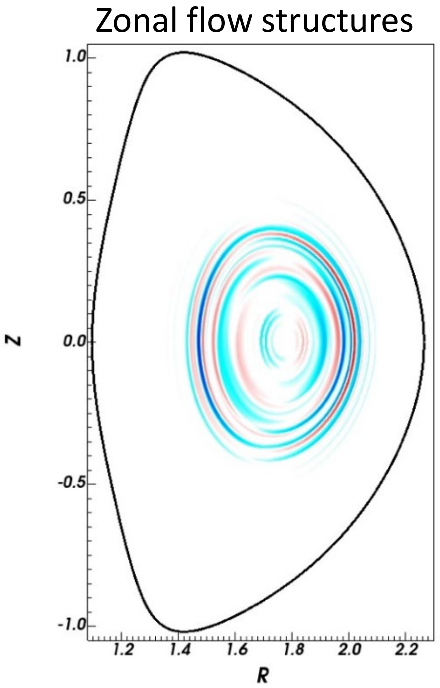
After startup transients, this shows dominant activity at ~100 kHz similar to experimental data

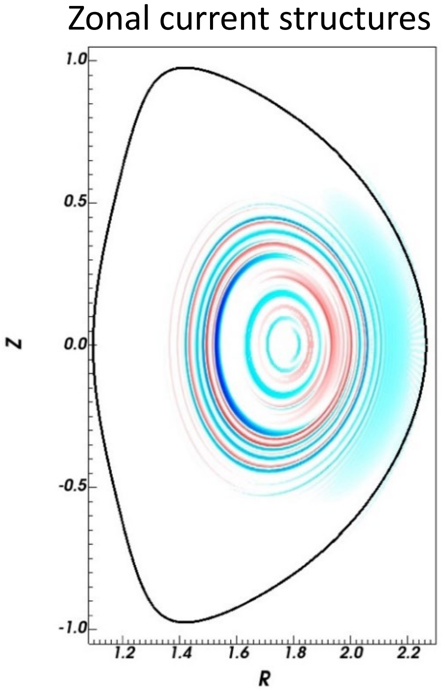


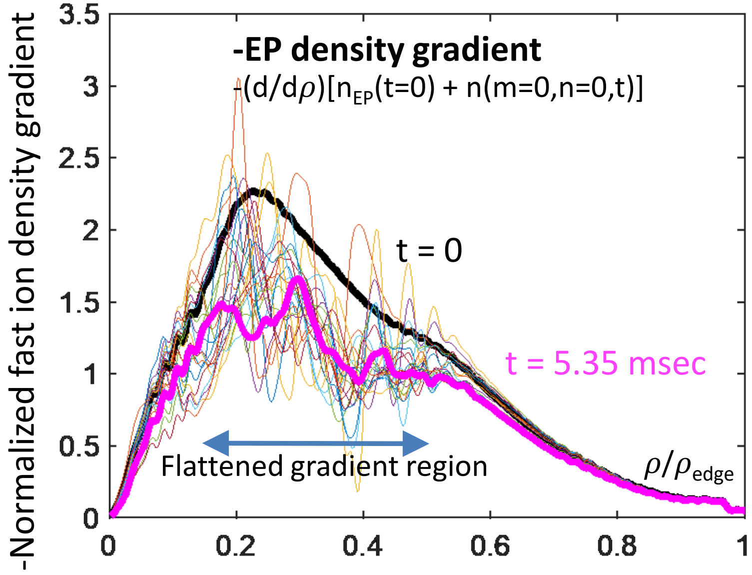
*D. A. Spong, M. A. Van Zeeland, W.W. Heidbrink, X. Du, J. Varela, L. Garcia, Y. Ghai, Nuclear Fusion **61** (2021) 116061.*

Long-time scale FAR3d nonlinear simulations demonstrate erosion of EP density gradient and role of zonal flow/currents in driving intermittency

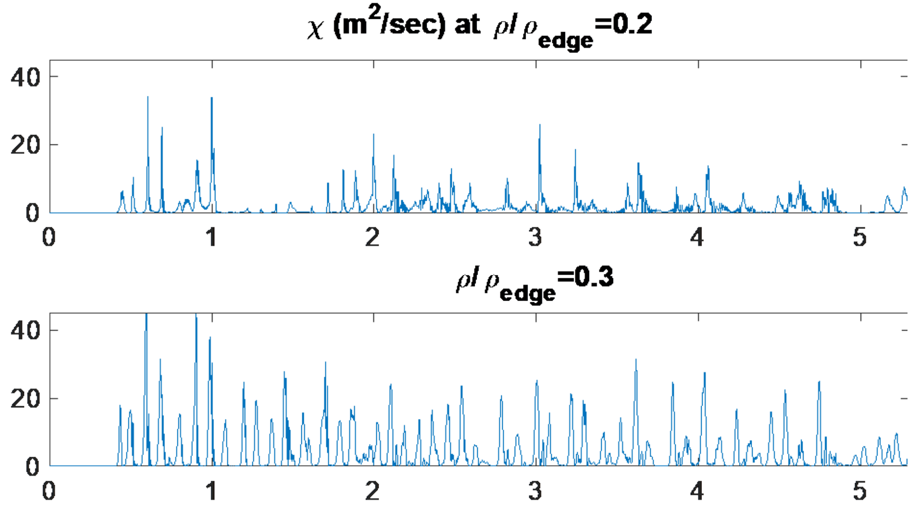




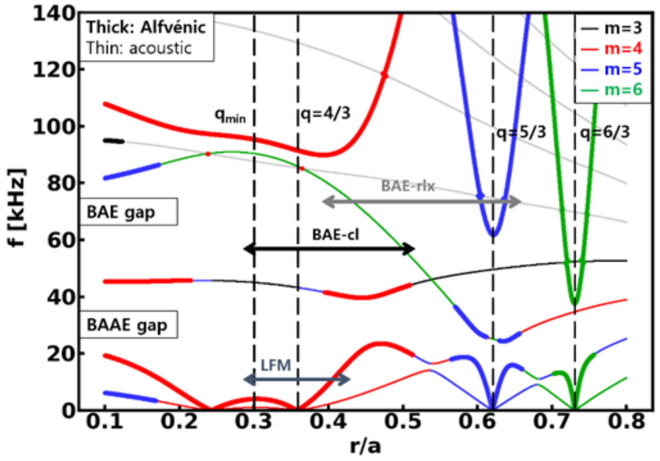




EP radial transport intermittency characteristics



GTC simulation of LFM/BAE instabilities in DIII-D elucidate the mechanism of the LFM and show LFM/BAE mode structures similar to experiment

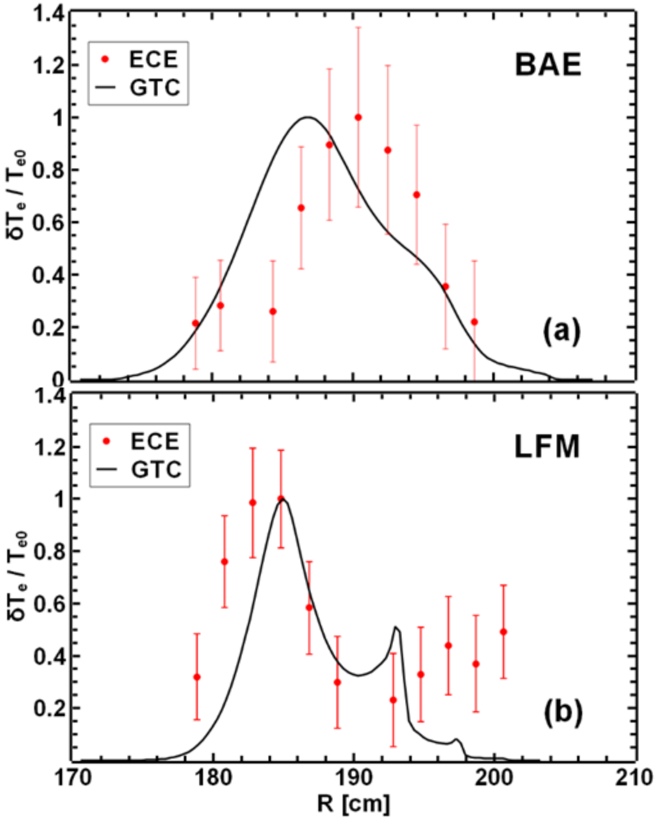


- **LFM** = **L**ow **F**requency **M**ode
  BAE = **B**eta Induced **A**lfven **E**igenmode

- GTC finds BAE with EP, and LFM without EP, consistent with DIII-D #178631

- Simulation finds LFM is an interchange-like electromagnetic mode excited by thermal plasma pressure gradient

- Compressible magnetic perturbations are crucial for BAE and LFM stabilities.



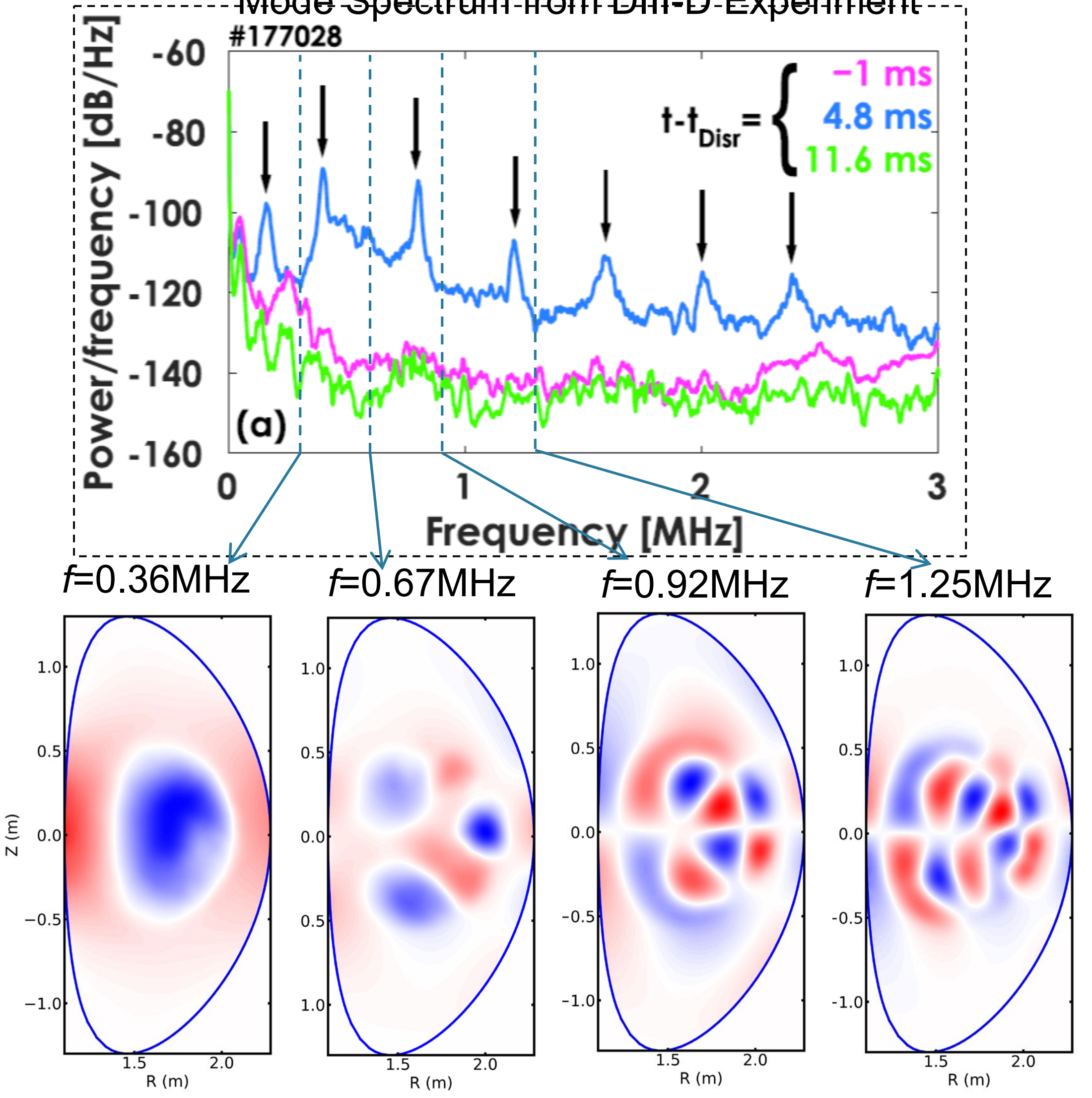
G. J. Choi et al, Nuclear Fusion 61, 066007 (2021)

M3D-C1 Simulation of Compressional Alfvén Eigenmodes excited by Runaway Electrons in Tokamak Disruptions

- Collaboration between ISEP & SCREAM
- M3D-C1-K identified current quench (CQ) MHz range modes observed in DIII-D disruptions as compressional Alfven eigenmodes (CAEs)
  - Mode frequencies agree qualitatively with experiments.
  - Mode is generated by trapped runaway electrons (REs)
    - Precessional resonance
    - momentum exchange via mirror force ($-\mu \nabla B$).
  - Strong correlation in experiments between CQ modes and RE beam formation
  - This simulation provides a reliable tool for the excitation of CAEs in disruptions and their mitigation effects on REs.

[C. Liu, APS DPP 2021 invited talk]

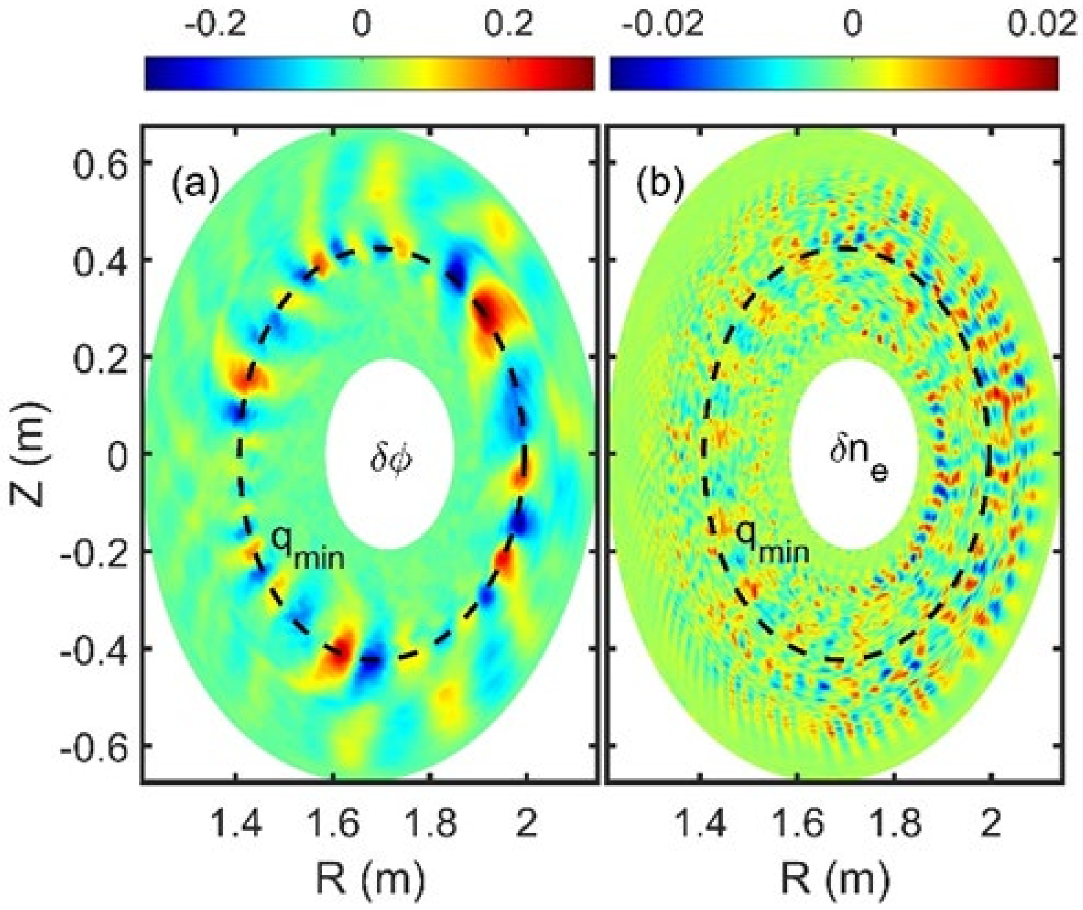
Mode Spectrum from DIII-D Experiment



Mode frequencies and structure from M3D-C1 simulation ($\delta B_{\parallel}$)

GTC simulation of ITG microturbulence regulates RSAE saturation & associated EP transport

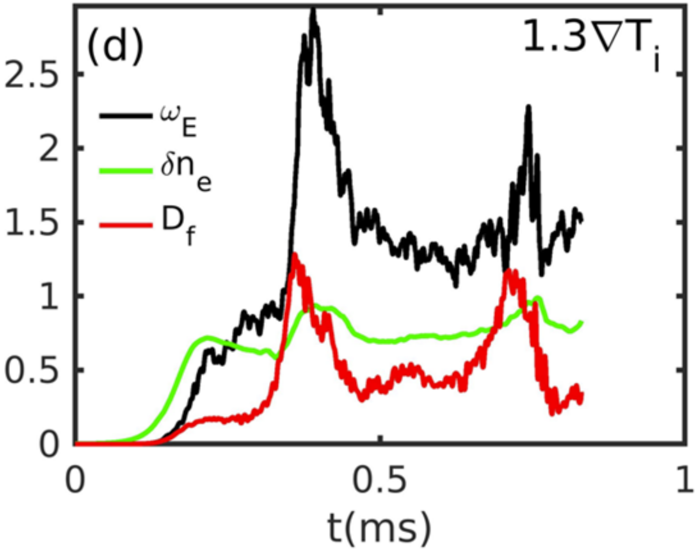
- n=[11,25] ITG reduces saturated RSAE amplitude & fast ion diffusivity
- Compared with ITG, RSAE has smaller δn_e but much higher $\delta\phi$
- Zonal flows mostly generated by RSAE
- RSAE turbulence maintain a quasi−steady state
- $D_f \sim 0.8\, m^2/s$ at late nonlinear stage close to experimental value



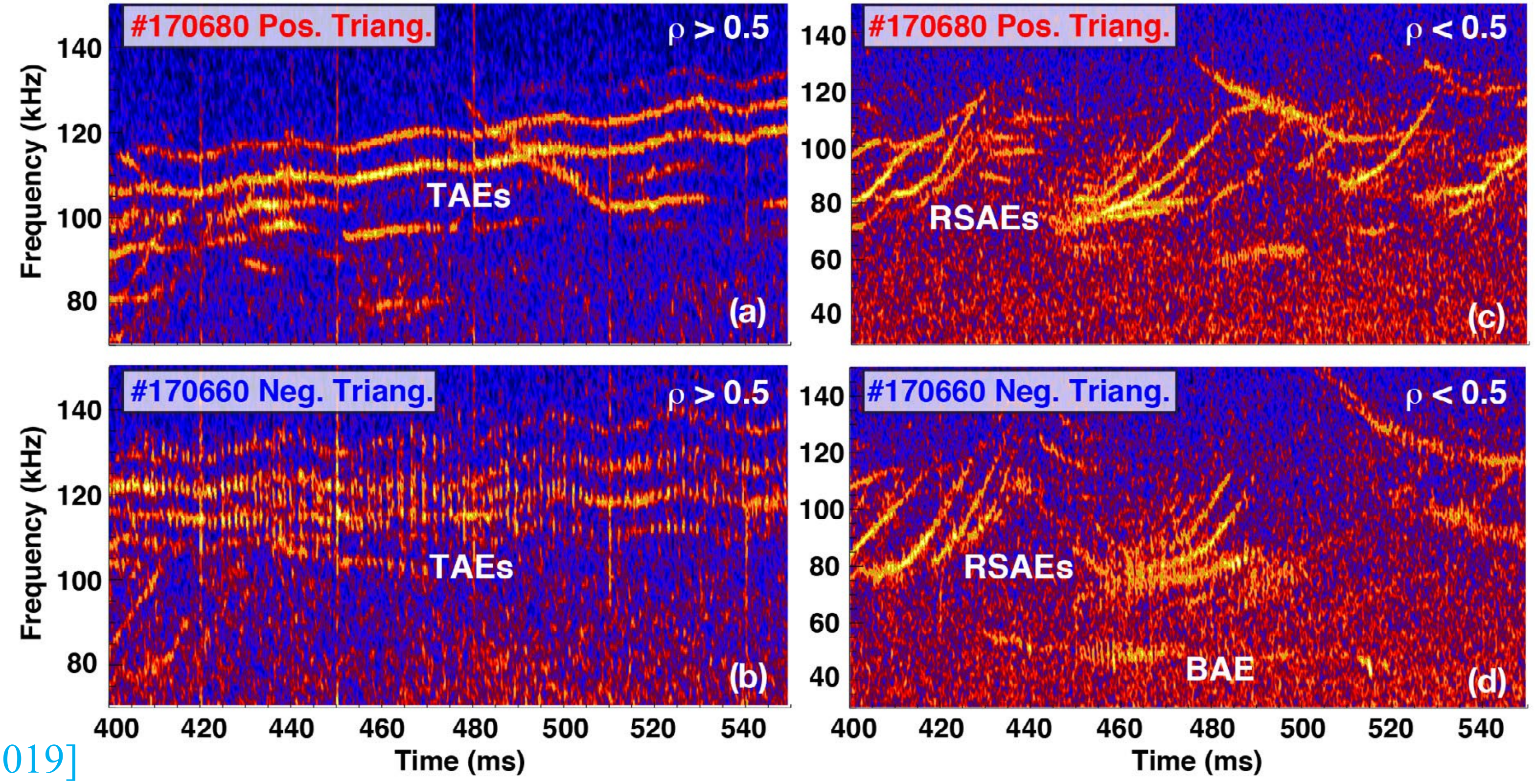
[P. Liu et al, submitted to PRL 2021]

GTC simulation shows EP transport intermittency induced by microturbulence regulation

- Intermittency in global kinetic-MHD simulations
  - → MEGA [Todo, NF2012]; FAR3D [Spong, 2021]. What leads to the repetitive burst?
- Chirping/intermittency present in negative triangularity DIII-D experiment [Van Zeeland, NF2019]
  - → RBQ model [Duarte, NF2017][Gorelenkov, PL-A2021]: enhanced chirping due to weaker ITG
  - → Intermittency induced by damping of ZF/ZS due to EP scattering by ITG [Liu , 2021]?



[P. Liu et al, submitted to PRL 2021]



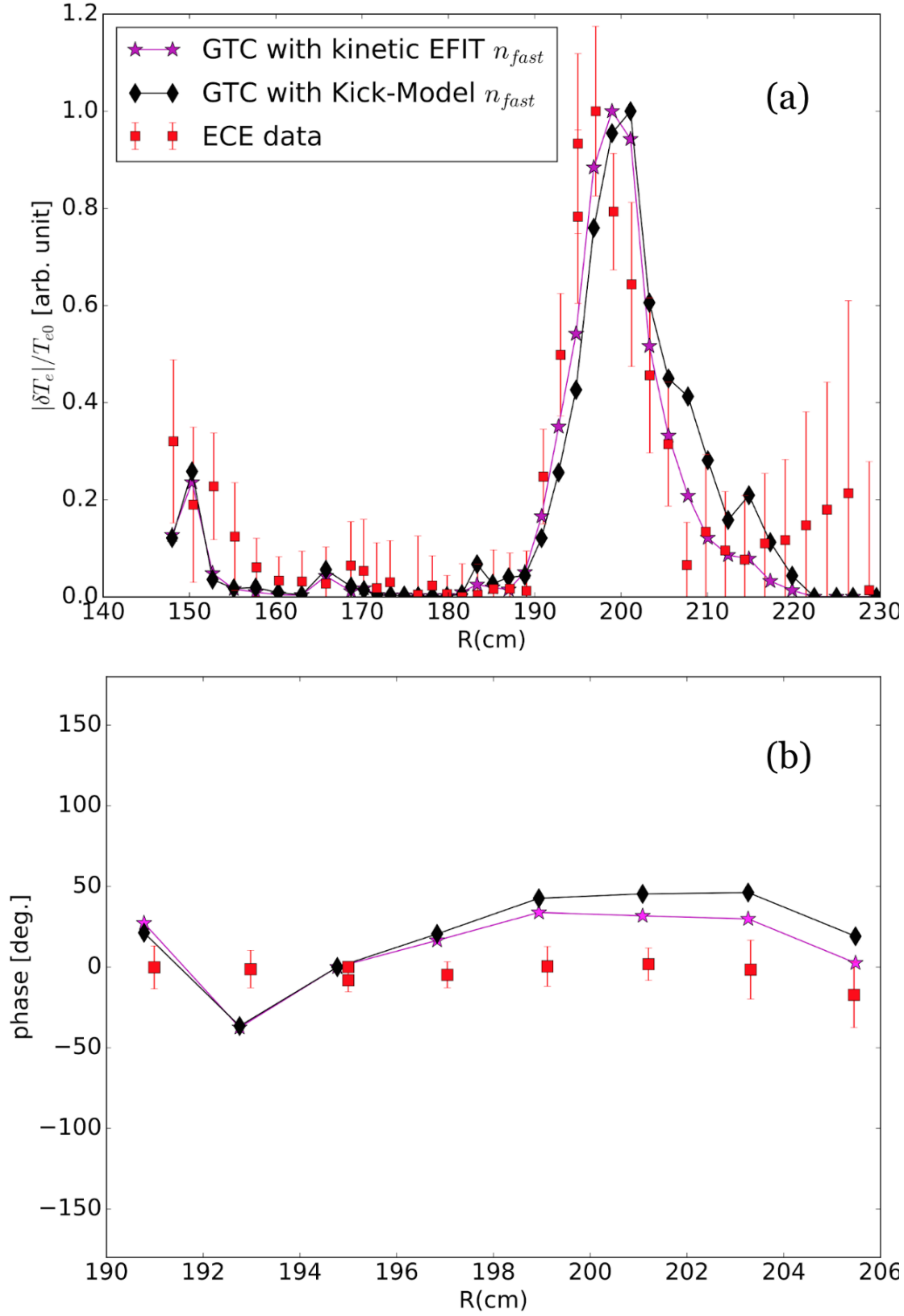
[Van Zeeland, NF2019]

GTC synthetic diagnostics show validation of mode structure

Comparison of GTC simulation of n=4 RSAE with experimental ECE data using Synthetic Diagnostic Platform [Shi, 2017].

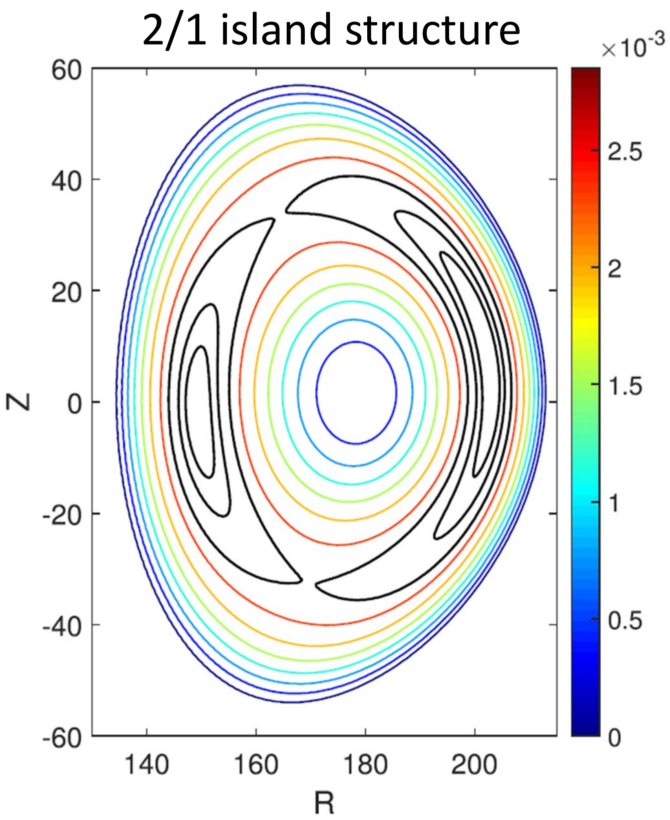
- Radial structure of δT_e
- The mode phase at R = 195.0cm.

[Taimourzadeh et al, 2018]



GTC simulates the interaction of EP with Neoclassical Tearing Mode (NTM) in DIII-D

- NTM island-induced EP re-distribution in DIII-D #157402
  - EP profile is partially flattened within 2/1 NTM island
  - stochasticity in phase space
- EP effect on NTM stability
  - Perturbed EP current has a weakly stabilizing effect on NTM stability
  - Consistent with observation that NTM island width decreased about 1 cm by fast ions.


2/1 island structure

Integrated EP density perturbation from 2/1 island

EP phase space distr. at μB_0 = 60 keV

[X. Tang et al, Phys. Plasmas 27, 032508 (2020)]

Summary

- ISEP has focused on EP components for integrated simulation and whole-device modeling
  - Long-time scale EP driven Alfvénic turbulence
  - Mesoscale couplings (ITG, RSAE)
  - Coupling between EP and thermal plasmas
    - Microturbulent regulation, intermittency
    - Neoclasssical tearing mode couplings with EP
  - Full range of frequencies (few kHz to MHz)
  - V&V starting point
- Future directions and critical unsolved problems
  - Full integration into whole-device modeling
  - EP transport predictive capability
  - ITER and FPP EP modeling
  - Application of machine learning methods

ASCR Partnerships Span Four Topics:

Workflows

Scott Klasky
ORNL, RAPIDS

GTC I/O Optimization
Workflow Automation
Analysis & Visualization

Linear Solvers

Rob Falgout
LLNL, FASTMath

GPU-accelerated
Algebraic Multigrid

Pathfinding

William Tang
Princeton

GTC-P Scalability
GTC-P Portability
FRNN Workflow
FRNN Scalability

Optimization

Samuel Williams
LBNL, RAPIDS

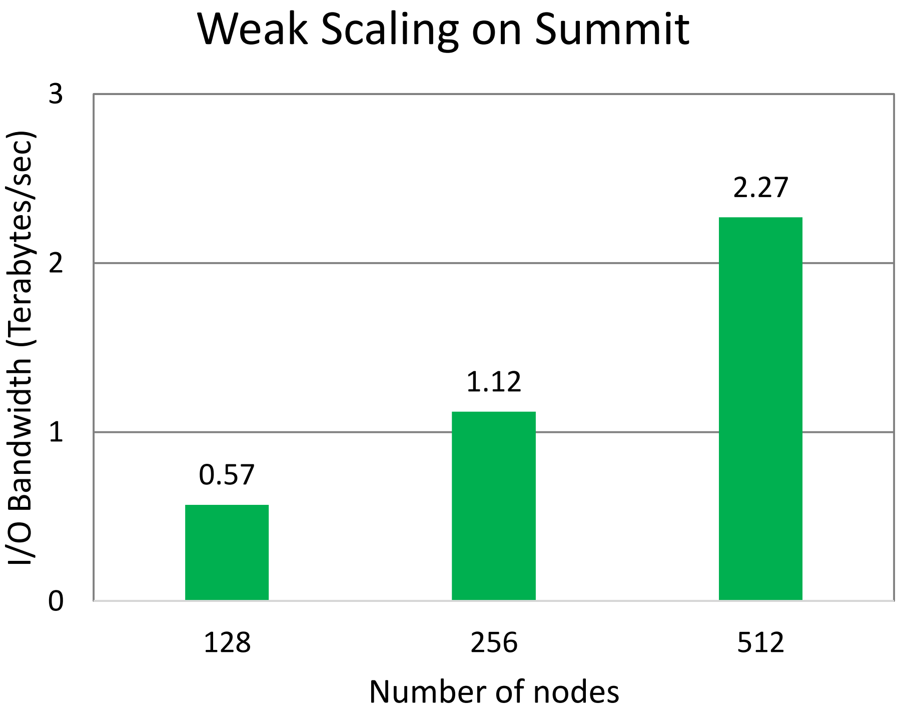
Performance Analysis and Optimization of GTC-P and FRNN

- ISEP funding was leveraged to integrate technologies and apply capabilities developed under the RAPIDS and FastMath SciDAC institutes.
- ISEP funding expanded/accelerated/specialized those core technologies.

ADIOS Integration / Optimization in GTC

- Under ISEP, ADIOS2 was integrated into GTC
- I/O optimized to reduce the overhead when running at scale
  - **Less than 5% overhead for I/O overhead when writing all of the output on the right**
  - **GTC was the “first full” application on Summit to sustain over 2 TB/s**

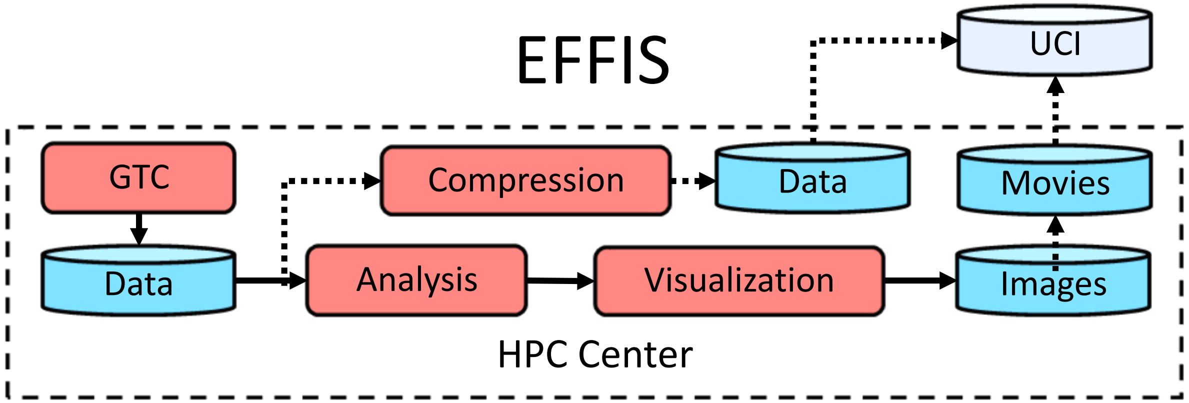
Output	ADIOS Dev Status
Equilibrium	✓
Data1d	✓
History	✓
Snapshot	✓
Phi3D	✓
Checkpoint-Restart	✓
Particle I/O	✓



L. Wan, K. Mehta, et al, “Data Management Challenges of Exascale Scientific Simulations: A Case Study with GTC and ADIOS”, ICCM 2019

Automating GTC Workflow with EFFIS

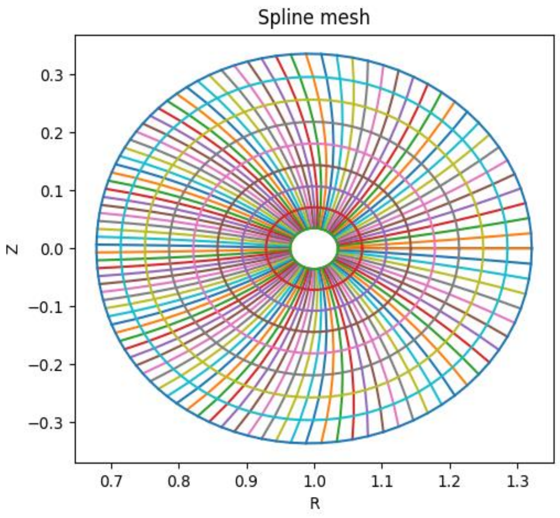
- EFFIS Framework
  - ○ Framework for coupled simulations and analysis
  - ○ Includes visualization and plotting services
  - ○ Remote dashboard for visualizing data

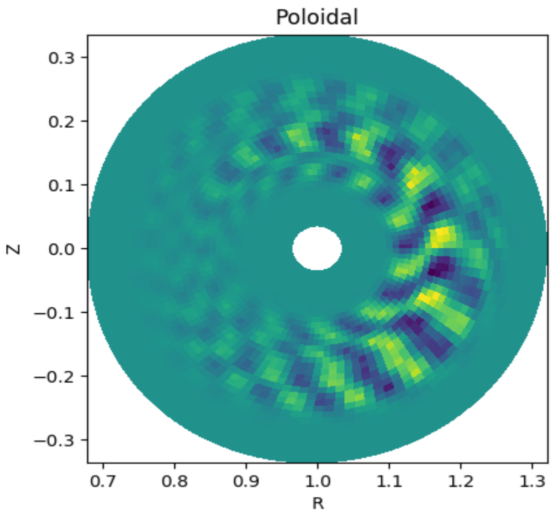


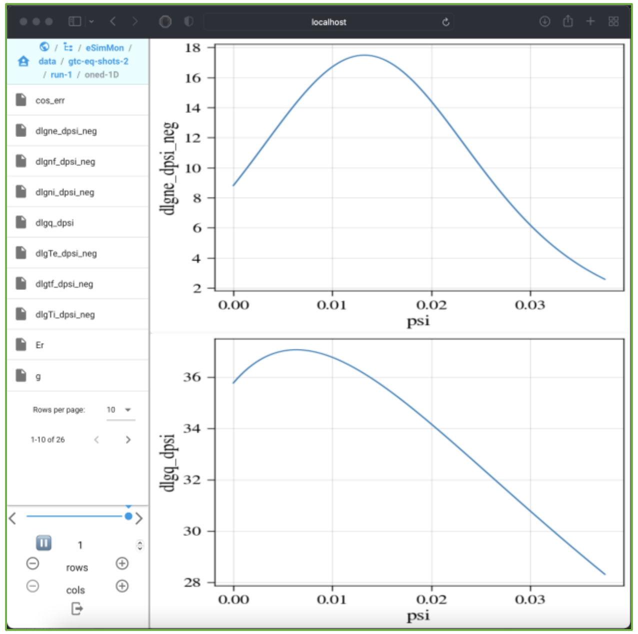
- GTC workflow was implemented in EFFIS
  - GTC scientists can compose their workflow in EFFIS using YAML
  - ➢ **in situ and/or post-processing can be scheduled, executed, and images migrated to UCI**
  - ➢ **Potential pathway for future Whole Device Modeling (WDM) coupler**

GTC Analysis and Visualization

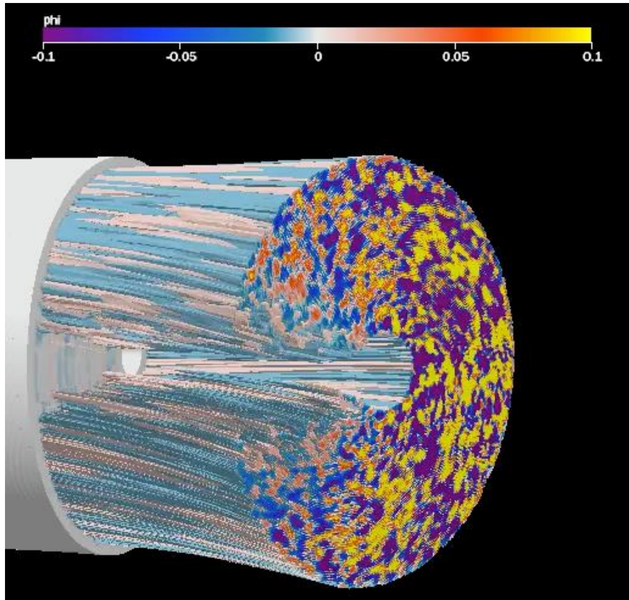
- Used VTK-M and ADIOS to:
  - Modify visualization of 1D & 2D quantities
  - Move from post processing to in situ
  - Create new 3D in situ visualizations of GTC
- eSimMon dashboard
  - Incorporated into EFFIS / GTC workflow
  - allows GTC scientist to monitor their simulations as they run





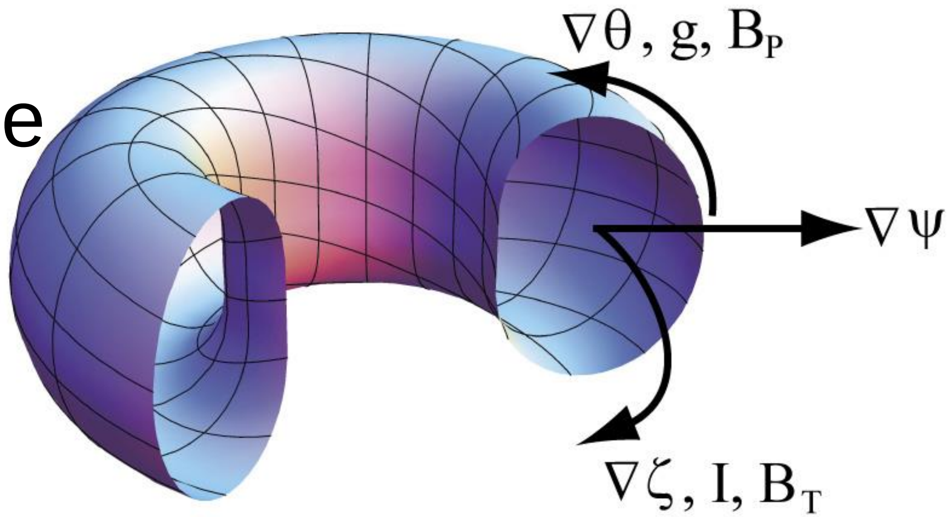


eSimMon Dashboard



Researchers can visualize GTC simulations in situ

Linear Solvers in GTC



- Particle-in-Cell methods (e.g. GTC) require a Poisson solve to calculate particle accelerations
  - Field solves can take as much as half the simulation time
- GTC uses HYPRE’s AMG solver
  - AMG solver is a scalable, grid-free method with O(N) complexity
  - Minimizing communication and setup costs are key to performance and scalability
- under ISEP, hypre effort focused on GPU-optimizations for AMG

GPU-enabled AMG cuts solve time by 3x

- GTC weak scaling DIII-D
  - 640K DOFs/MPI
  - LLNL’s Lassen (2x22c P9 + 4xV100)
  - 4 MPI processes per node (10 cores + 1 GPU per MPI)

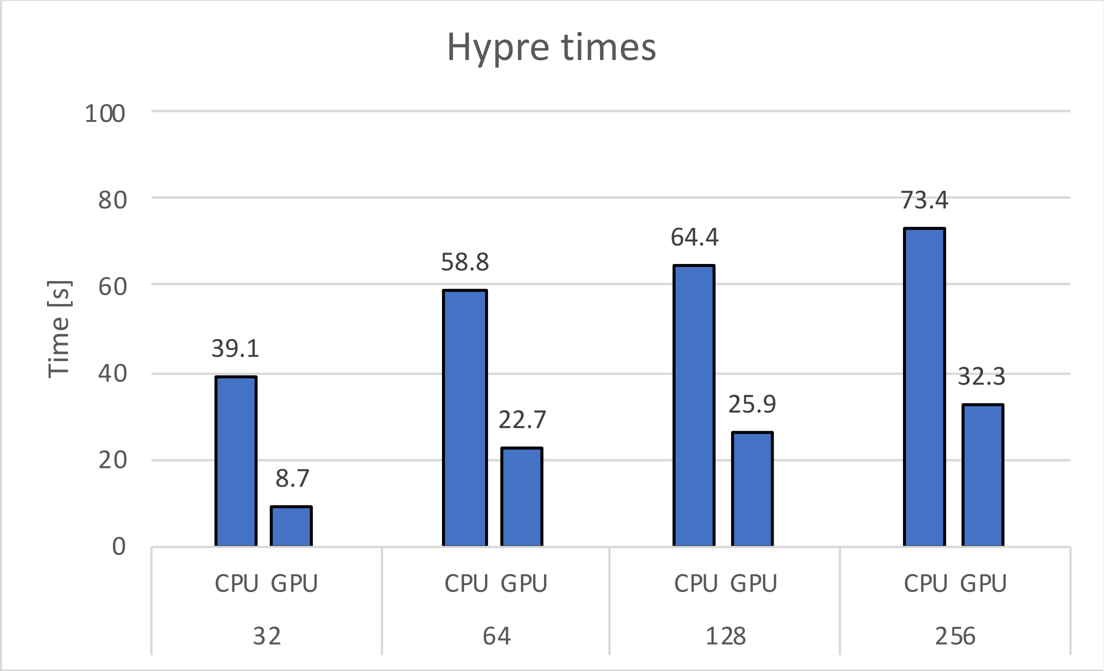
- GTC Poisson dominated CPU time
- Through ISEP, hypre setup and solve run entirely on the GPU

➢**GPUs can reduce hypre time by 3x**

➢**GTC still has sizable Poisson time outside of hypre**

Poisson Dominates

Poisson time outside hypre



GTC-P Optimization and Analysis

- GTC-P is a reduced & simplified version of GTC
  - Used as a proxy app to prototype performance, scalability, and portability solutions for GPUs and manycore CPUs before integrating into GTC

- Intel / KNL Optimizations
  - William Tang (PPPL, PU), Bei Wang (PU)
  - NERSC/TACC processor with fast (MCDRAM) and capacity (DDR) memories
  - Developed novel solutions for partitioning particle and grid data

  ➢ **Pass along GTC-P best practices (optimizations and FOM) into GTC (e.g. time-to-solution, radial sorting, etc…)**

- NVIDIA GPU Analysis
  - Samuel Williams, Khaled Ibrahim, Protonu Basu (LBNL)
  - KNL(Cori) and GPUs (Summit)
  - NVProf issues stalled GPU analysis
  - GPU issues resolved with Nsight compute; personnel had left by that point

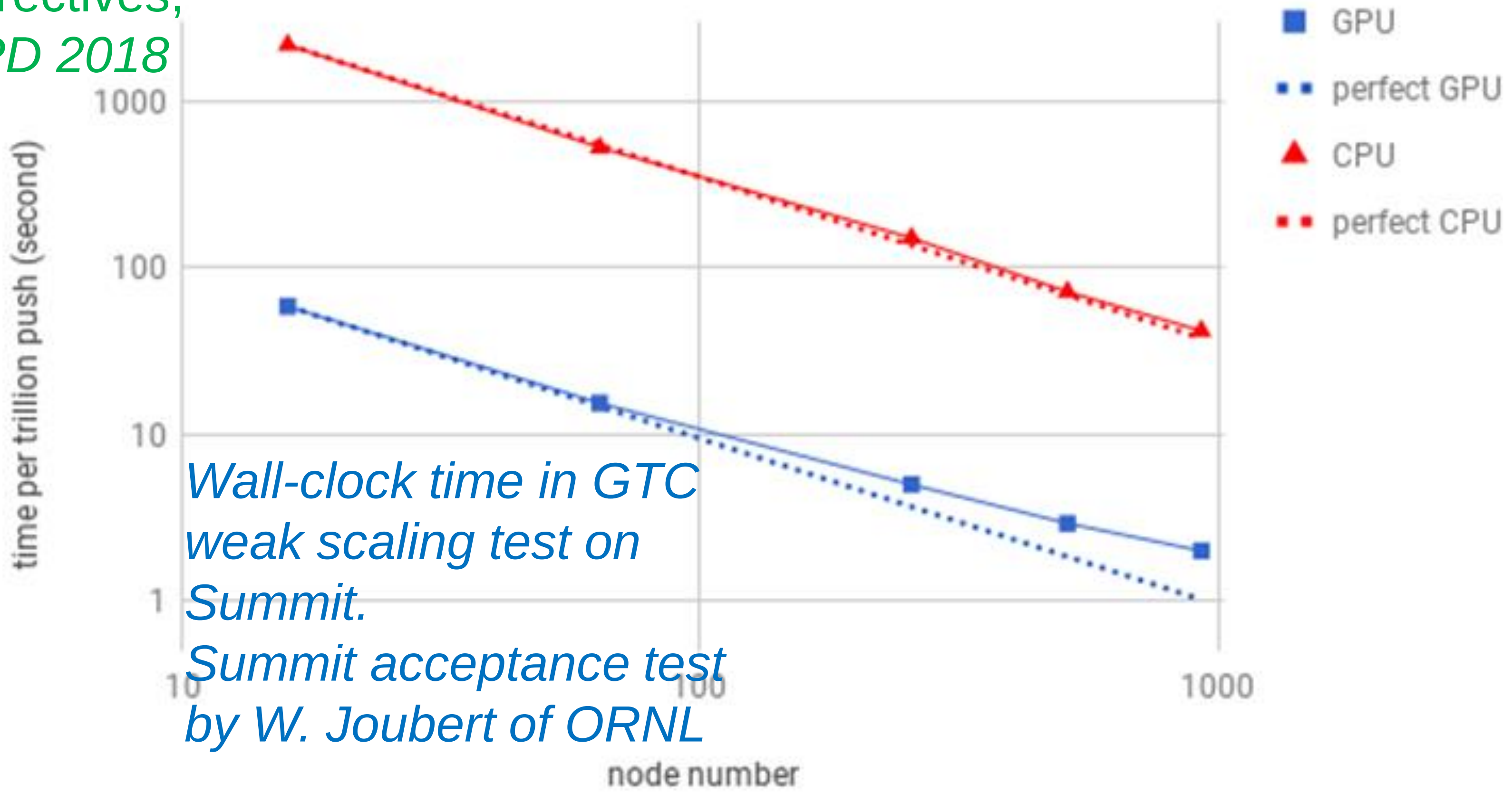
  ➢ **Most functions (except shift_t) insensitive #GPUs/node.**

  ➢ **Caches are mostly insensitive to grid size and density**

Utilization of the Summit GPUs has provided significant performance gains for GTC

- GPU optimization by ISEP & CAAR projects
- GTC speeds up 40x from CPU to GPU on 384 GPUs; speeds up 20x from CPU to GPU on 5556 GPUs (1/5 of SUMMIT)

Heterogeneous Programming and Optimization of Gyrokinetic Toroidal Code Using Directives, Wenlu Zhang et al, [*SC2018, WACCPD 2018 Workshop*]



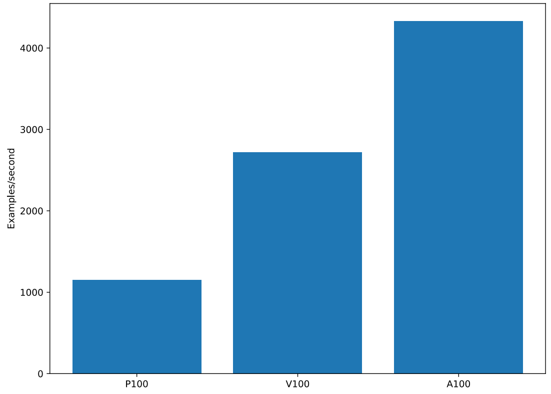
Wall-clock time in GTC weak scaling test on Summit.

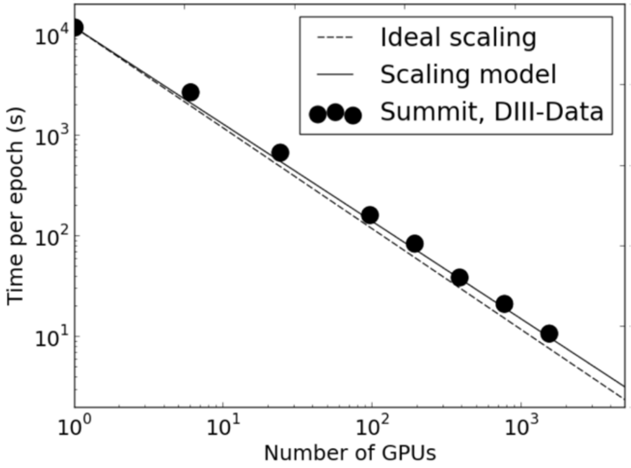
Summit acceptance test by W. Joubert of ORNL

Using DL to Predict Disruptions

- FRNN is used to predict disruptions in tokamak plasmas

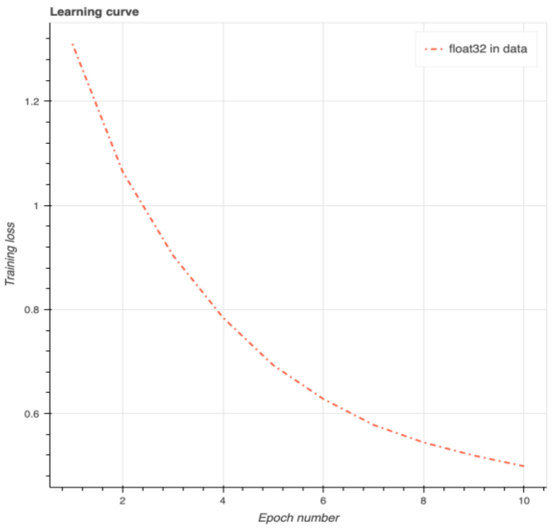
- Scalability and Performance
  - Bill Tang (PU), Ge Dong (PU), Kyle Felker (ANL)
  - generation over generation gains on GPUs
  - **DIII-D training scales to over 1000 GPUs**

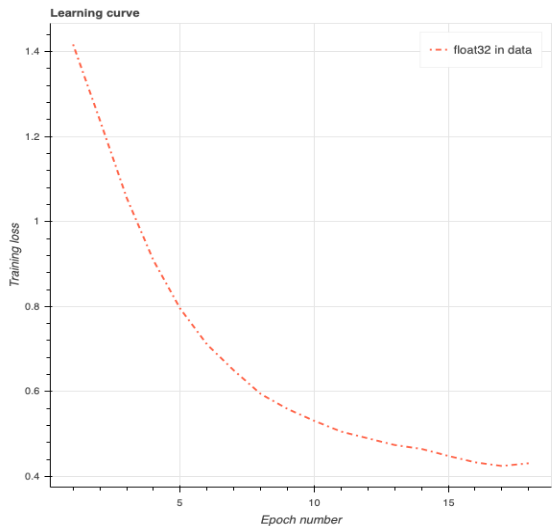




J. Kates-Harbeck, A. Svyatksovkiy, W. Tang, “"Predicting Disruptive Instabilities in Controlled Fusion Plasmas through Deep Learning”, NATURE, April 2019.

- Performance Analysis
  - Collaboration with Princeton, Matt Leinhauser (U.Del, summer intern at LBL)
  - Cori GPU (V100) and Spock (MI100)
  - Number of SW issues on Spock
  - **MI100 was about 1.38x faster**





ASCR-FES Collaborations

Telecons/Meetings

- semi-weekly ORNL-UCI zoom
- ORNL-led training on GTC+EFFIS workflow; ADIOS+GTC Python analysis; ADIOS hackathon
- LLNL-UCI (Victor Magri and Xishuo Wei) person-to-person interactions
- Monthly (semi-weekly in summer) LBL-Princeton-ANL telecons on FRNN in 2021
- ISEP AHM and workshops

Publications

- L. Wan, et al., “Data Management Challenges of Exascale Scientific Simulations: A Case Study with GTC and ADIOS”, ICCM 2019.
- R. Falgout, et al., “Porting hypre to heterogeneous computer architectures: Strategies and experiences”, Parallel Computing, 108, 2021. LLNL-JRNL-816235.
- W. Tang, et al., "Implementation of AI/Deep Learning Disruption Predictor into a Plasma Control System", IAEA Fusion Energy Conference, Oral Paper TH-7, Virtual Conference, 2021.
- G. Dong, et al., "Deep Learning Based Surrogate Model for First-Principles Global Simulations of Fusion Plasmas", (accepted), Nuclear Fusion, 2021.
- G. Dong, et al., "Fully Convolutional Spatio-temporal Models for Representation Learning in Plasma Science", Journal of Machine learning for Modeling and Computing, 2021.

Plans for ISEP Year 5

Workflows & I/O

- NVMe optimization
- Visualization of Stellarator and particles

hypre / Algebraic Multigrid

- Solver optimizations for Perlmutter (NVIDIA A100) & Frontier (AMD MI200)

Pathfinding

- FRNN workflow & performance scalability on Summit, Theta-GPU, Perlmutter, Cori, Spock,
- SGTC development (DL surrogate simulator for the ISEP GTC code) for real-time forecasting of key EM instabilities

Performance optimization

- FRNN performance analysis on Perlmutter (NVIDIA A100) & Frontier (AMD MI200)
- GTC-P performance analysis and optimization on Perlmutter and Frontier

Future Directions

- Workflows & I/O
  - I/O, DAOS, Frontier, Perlmutter optimizations
  - Workflow integration with Python notebook
  - Push towards coupling for Whole Device Modeling
- DL and Surrogate Modeling
  - Leverage Deep Learning technologies to predict plasma instabilities and disruptions
  - Create surrogate models that provide low-latency prediction of instabilities and disruptions
  - Evaluate/Compare DL/surrogate techniques as a sidecar for real-time plasma control systems
- hypre / Algebraic Multigrid
  - Solver performance for 3D field Poisson model in GTC
  - GPU-enabled hypre in other ISEP codes, e.g., GYRO and FAR3d
- CS/Math/Fusion CoDesign
  - PIC methods are limited by #particles and #time steps.
  - Future HPC computing resources will not increase as fast as in the past (continue to be specialized for AI/GEMMs/reduced precision)
  - How can GTC do significantly more science with moderately more HPC compute resources?

Review the critical gradient model (CGM)

- **V&V physics basis of the CGM was developed with SciDAC EP funding (2008-2017)***
  - ► The CGM was developed from multi-scale GYRO local nonlinear simulations of EP-driven low-n AE modes embedded in high-n microturbulence.
  - ► The GYRO simulations showed EP transport becomes unbounded beyond a critical EP density gradient.
  - ► A recipe was derived giving the AE linear threshold for unbounded transport and coincident critical EP density gradient profile.
  - ► A stiff critical gradient transport model in a EP density transport code provides the EP transport flows quickly.

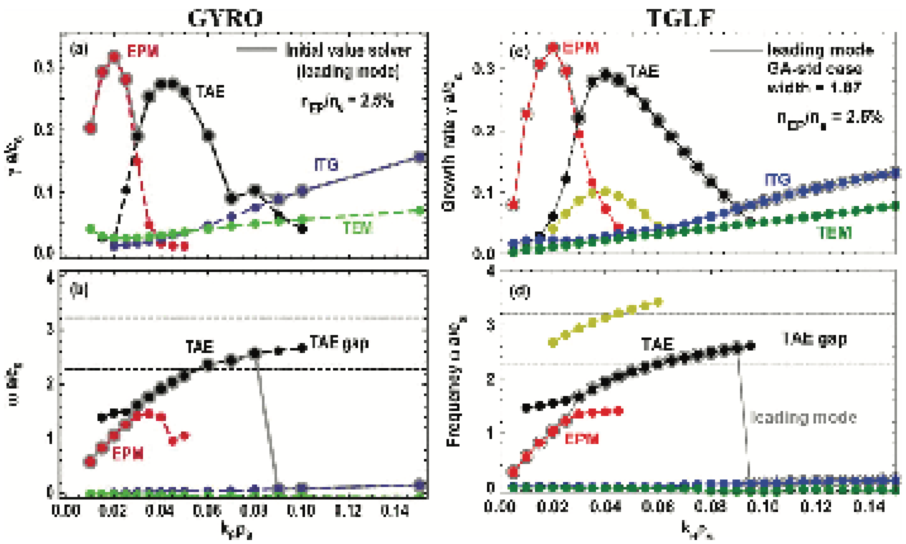
  - The main goal of the reduced physics CGM is to make an EP module for quickly computing the AE-EP transport flows and plasma heating losses.

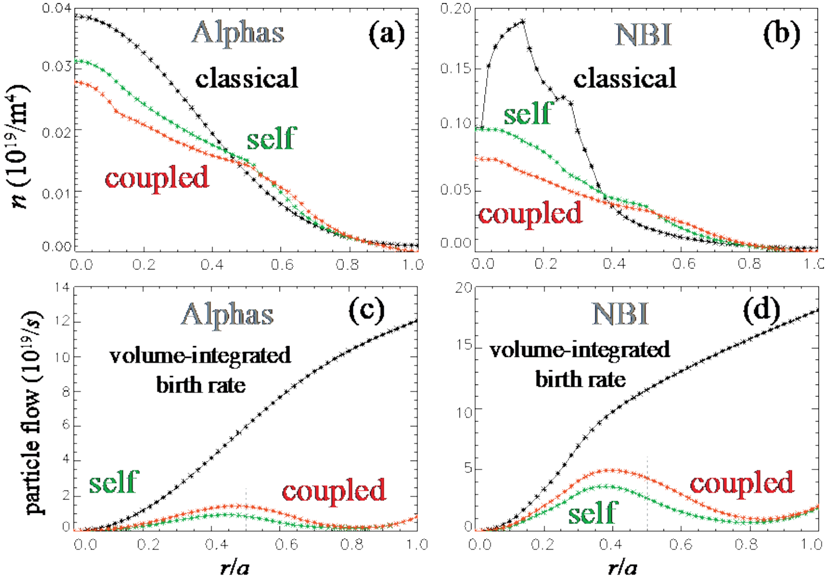
    The EP module will be integrated into the SciDAC Atom2 WDM project.

- **Major CGM accomplishments in last 4-years**
- **Work in progress and remaining goals**

* APS-DPP invited talks: 2009, 2013, 2016

Prediction of Alfvén eigenmode energetic particle transport in ITER scenarios with a critical gradient model *





- Our latest CGM EP transport code uses a gyrofluid code TGLF-EP rather than GYRO. The new coding automatically gets the AE-threshold and critical gradient profile much faster.

- Our 2014 ** first ITER projections use slow “by hand” GYRO runs whereas the 2018 projection with the faster TGLF-EP now treats the fusion Alpha transport with added coupling to 1Mev NBI AE-EP transport.

- The AE’s only transport a small fraction of birth EP’s to the edge (r/a > 0.8) where the GYRO fitted microturbulence model transports only the low-energy EP’s escaping the plasma.

- CGM model showed low-current (steady state) ITER scenarios have much larger fractions of the birth EP’s escaping the core to the edge than the high-current scenario (above), and significantly more if the current was not given time to penetrate…….. All consistent with modeling DIII-D experiments.

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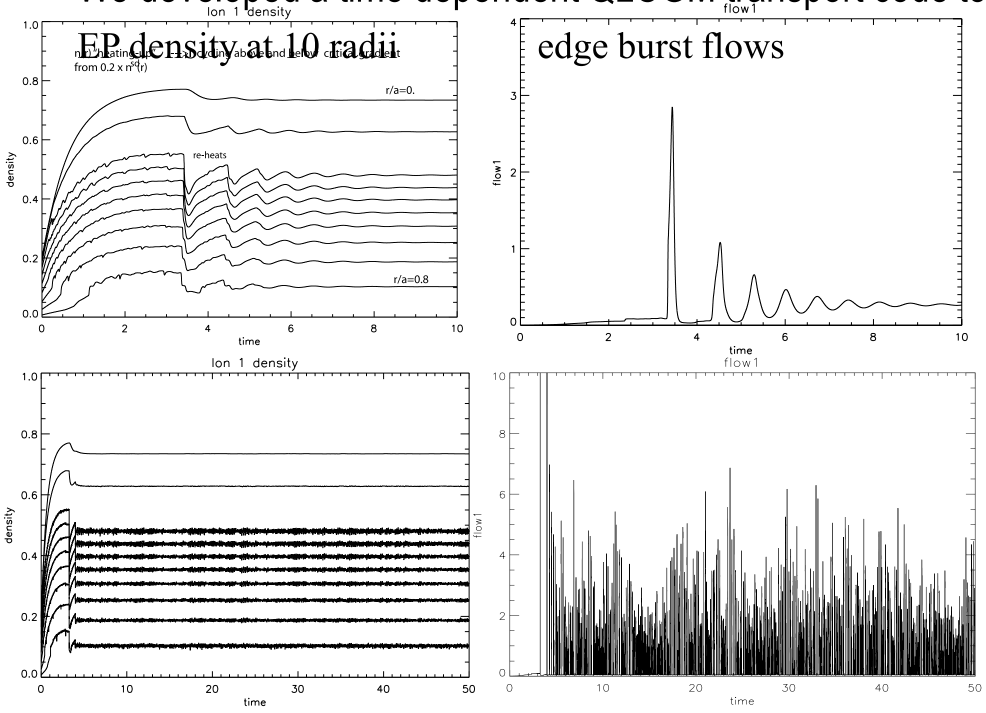
* E.M. Bass and R.E. Waltz, Nucl. Fusion 60 (2020) 016032 (2018 IAEA-FEC oral)

** R.E. Waltz and E.M. Bass, Nucl. Fusion 54 (2014) 104006 (Bass 2013 APS invited)

Quasilinear critical gradient model (QLCGM) for the intermittency of Alfven eigenmode transport of energetic particles*

- Intermittency is a measure of burstiness in a time signal.
  Highly intermittent EP flows escaping the plasma may increase wall erosion.
  The DIII-D fast ion loss detector (FILD) has a noisy signal with an intermittency O(1.4) increasing with source power.
  This suggests AE-EP transport has 10x intermittency simulated microturbulent transport O(0.14).
  High intermittency is a feature of stiff transport near a critical gradient.

- We developed a time dependent QLCGM transport code to follow the avalanching transport and bursting EP edge.



- The avalanching limit cycle burst flows decayed.

  Alfven modes damp on the thermal plasma which has a lot of noise from microturbuence.

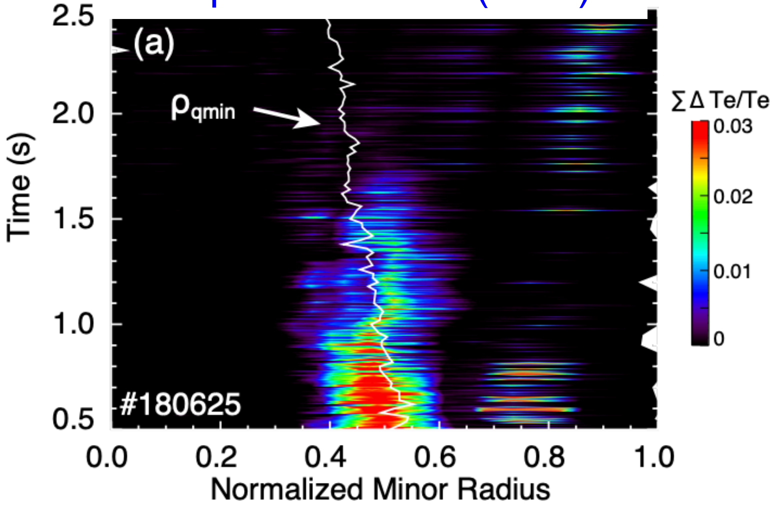
- When DIII-D microturbuent noise level was added to the DIII-D AE damping rate , the QLCGM transport code with matching parameters found noisy edge burst with intermittency O(1.4) increasing with source power matching DIII-D.

- These are Quasilinear transport simulations.
  Nonlinear simulations will add another source of intermittency from direct mode-mode coupling.

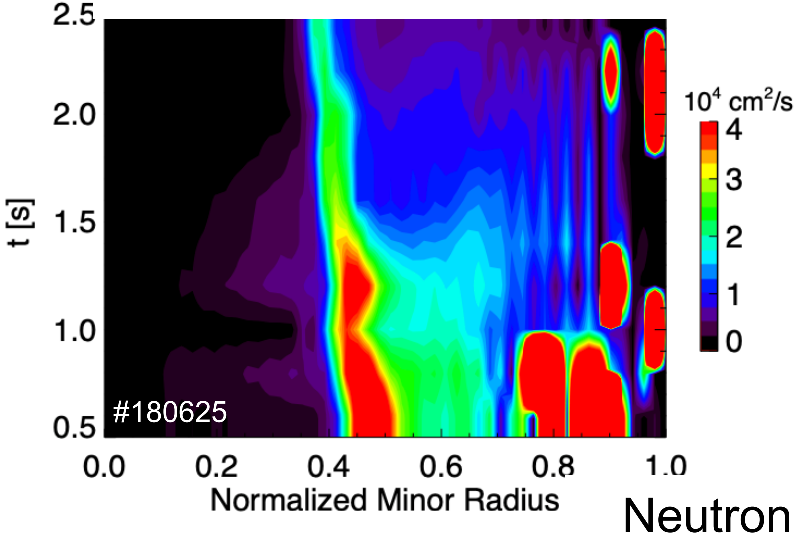
*R.E. Waltz, E.M. Bass, C.S. Collins , and K. Gage, Nucl. Fusion 61 (2021) 036043

Improving fast-ion confinement and performance by reducing Alfven eigenmodes in the q-min >2 steady experiment scenario

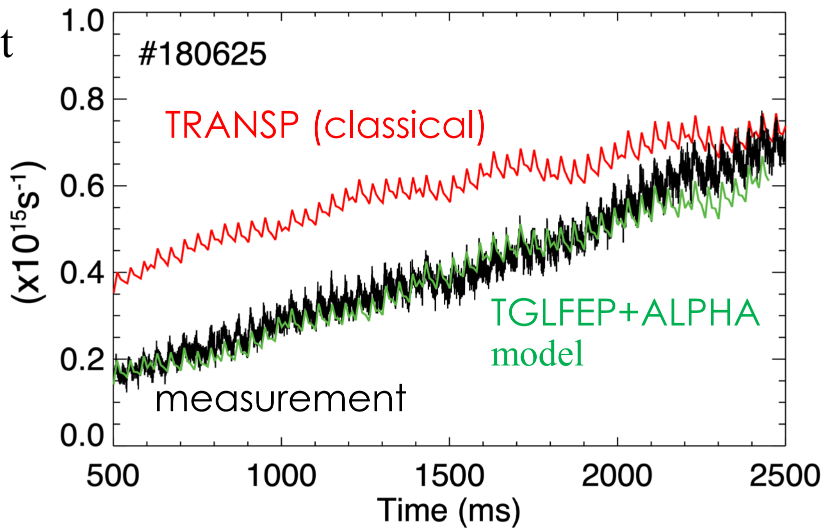
Experiment AEs (ECE)



Model Diffusion Prediction



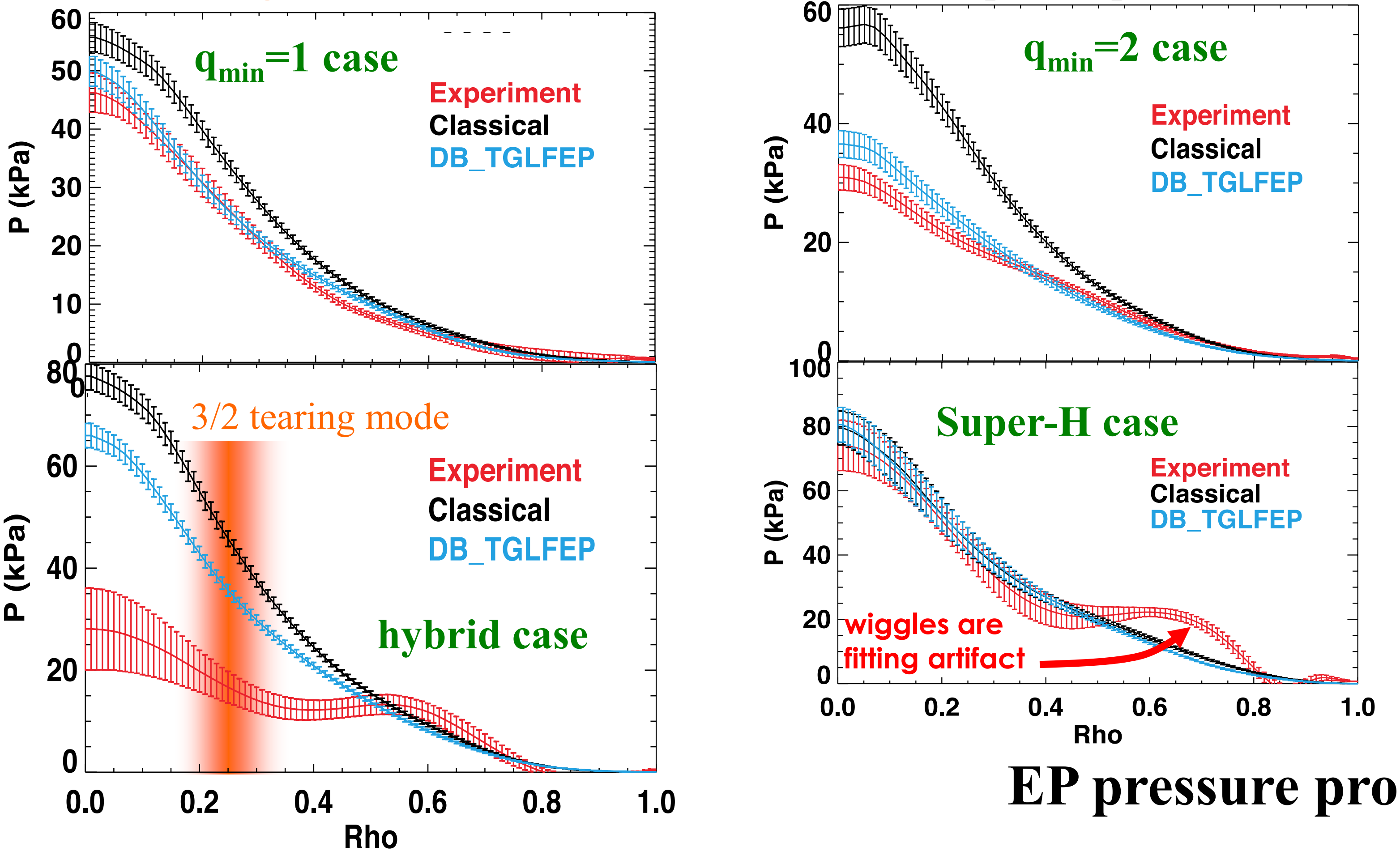
Neutron Rate



- TGLF-EP+Alpha **predicts** the AE diffusion coefficient without any inputs from **experiments** with good agreement over the whole current ramp-up.
- The diffusion coefficient is added to TRANSP for a **neutron prediction** in spectacular agreement with **experiment**, over a wide range from heavy EP transport to nearly **classical**.

Validation of the TGLF-EP+Alpha model in DIII-D scenarios for ITER

Single time slice validations have been performed for a diverse group of ITER-relevant DIII-D scenarios, with **generally good agreement** except in the “hybrid” case where a destructive **tearing mode** (unaccounted for in TGLF-EP+Alpha) is present



EP pressure profiles

E.M. Bass, M. A. Van Zeeland, R. E. Waltz, “Validation of the TGLF-EP+Alpha model in DIII-D scenarios for ITER”, Nucl. Fusion paper in progress

Work in progress and remaining goals

- A Global Quasilinear Critical Gradient Model (GQLCGM) based on GYRO global modes is in progress.

  _The CGM has been based on local AE modes rather than global modes.

  _An EP transport code has been coupled into global GYRO. This allows global AE modes to quasi-linearly relax to a global critical gradient profile.
  How well does this global CGM profile compare to the local CGM profile?

- Our longstanding goal has been to develop an EP module or work flow so that the fast reduced physics CGM approach can be integrated into WDM standard transport codes. Non-expert EP plasma transport modelers can then easily include the currently ignored AE-EP driven transport losses in standard experimental analysis and ITER projections.

- With the success of the TGLF-EP AE-EP linear growth rates accurately matching GYRO and alternative short-cut to our goal with less reduced physics may be possible.

_ We will try direct use of TGLF (module in Atom2 WDM) to find the low-n AE-EP driven losses along with the high-n microturbulent losses TGLF was designed to treat.
_ Will this approach match the CGM EP density and transport loss profiles?

Papers and selected oral presentations 2017-2021

- ►E.M. Bass (UCSD), R.E. Waltz (GA), “Prediction of Alfvén eigenmode energetic particle transport in ITER scenarios with a critical gradient model”, Nucl. Fusion 60 (2020) 016032. IAEA-FEC 2018 selected oral

- ►R.E. Waltz, E.M. Bass, C.S. Collins (GA), and K. Gage (UCI), “Quasilinear critical gradient model for the intermittency of Alfven eigenmode transport of energetic particles, Nucl. Fusion 61 (2021) 036043

- ►C.S.Collins, C.T. Holcomb (LLNL), M.A. Van Zeeland (GA), E.M. Bass (UCSD), “Improving fast-ion confinement and performance by reducing Alfven eigenmodes in the q-min >2 steady experiment scenario”, Nucl. Fusion paper in progress , IAEA-FEC May 2021 selected oral.

- ►E.M. Bass, M. A. Van Zeeland, R. E. Waltz, “Validation of the TGLF-EP+Alpha model in DIII-D scenarios for ITER”, Nucl. Fusion paper submitted

Fast ion relaxation in (i) Resonance Broadened Quasi-Linear (RBQ), (ii) kick reduced models and NTM AI/Machine Learning model (iii) Fusion Recurrent Neural Network (FRNN)

One ISEP SciDAC goal is to develop numerically efficient reduced models

RBQ: N.N. Gorelenkov, *V.N. Duarte (PPPL, ISEP - former Postdoc)*

kick: *M. Podesta (PPPL, ISEP)*

FRNN: *W. Tang, Ge Dong (PPPL, ISEP - Postdoc)*

in collaboration with
H.L. Berk (IFS, ISEP), R. White (PPPL),
J. Lestz (UC Irvine - PPPL graduate), M.V.Gorelenkova (PPPL)

FES SciDAC partnerships for ISEP SciDAC, October, 2021

Work is supported in parts by ISEP SciDAC

RBQ1D code started in year 1 of ISEP SciDAC

RBQ is a post- (NOVA/NOVA-K) processor to compute EP dynamics in the presence of Alfvénic modes.

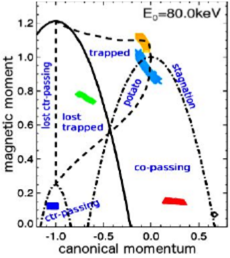
- RBQ includes:
  - eigenmode structures (NOVA or other solvers);
  - finds Alfvénic Eigenmode (AE) amplitude evolution and EP distribution in time;
  - Quasi-linear (QL) model is based on the diffusion in Constants of Motion space ⇒ oscillations/intermittences!!
- RBQ is connected with TRANSP Whole Device Model to compute EP diffusion and distribution function *(Gorelenkov et al., NF'18).*
- Extensively ***V&V against existing/developed analytic*** cases *(Gorelenkov et al., APS'18, Duarte et al. APS'20).*
  - WPI resonances are studied in COM using ORBIT *(Meng et al.,NF'18, White et al., PoP'18).*

RBQ aims at single, multiple AE instabilities expected in BP conditions given its efficient calculations.

(2) Kick (reduced) model existed prior to SciDAC & recent development in kick model

- Mostly *interpretive* analysis: mode properties known from experiment
  - Mode spectrum (frequency, mode numbers), estimates for amplitude
- Model tested for single-mode and multi-mode scenarios
  - Targets: NSTX/NSTX-U, DIII-D, KSTAR, TCV, JET, …
  - AEs, NTMs, sawteeth, … - only one type of perturbation
  - AEs + kinks/fishbones
  - AEs + NTMs
  - NTMs + kinks

- Also tested for *predictive* analysis of EP-driven modes (TAEs, RSAEs)



Kick model is based on ORBIT guiding center simulations

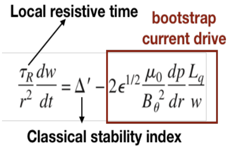
Improved ORBIT outputs for stand-alone analysis; used in subsequent NUBEAM simulations

Can use GPU optimized ORBIT version

<—— examples of fast ion diffusion in COM space

FRNN (fus.recur.neur.network) AI/DL model was also started at the start of ISEP

- Input signals for physics-based reduced models of **Neoclassical Tearing Modes (NTM's)** is collected;
  It is integrated into FRNN Machine Learning workflow for predicting tokamak disruptions.
- Signals include (i) pressure gradient profiles (proportional to the bootstrap current), (ii) rational surface locations, and (iii) measured islands captured in a "Reduced Model"
  - See Sam Williams presentation for more details.

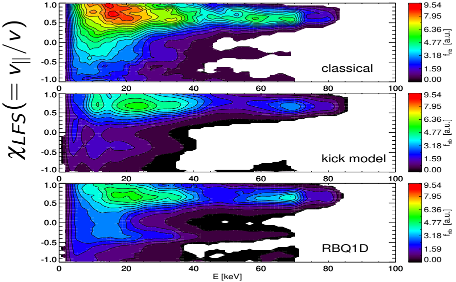


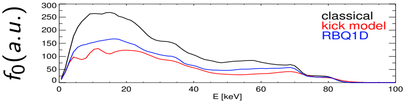
$$\frac{\tau_R}{r^2}\frac{dw}{dt} = \Delta' - \boxed{2\epsilon^{1/2}\frac{\mu_0}{B_\theta^2}\frac{dp}{dr}\frac{L_q}{w}}$$

FRNN ML workflow improves ***disruption*** predictions.

New quasi-linear RBQ and a kick model have similar distribution functions

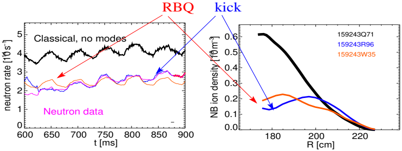
DIII-D shot #159243 was processed by NUBEAM TRANSP whole device modeling with RBQ or kick diffusion coefficients.





- Co-going passing ions are strongly redistributed.
- Amplitudes are kept constant

  throughout observed times.
- Neutron rate includes radial and energy dependence within TRANSP simulations.
- (Near) hollow EP density is due to COM core location sensitive diffusion.



Generalization of 1D RBQ model to 2D QL theory in COM space

- Employ the action-angle formalism for 2D Quasi-linear theory:
  (Kaufman,PhFl'72, Berk,Breizman, NF'95, Gorelenkov, PoP'19)
- Distribution function f is evolved by 2D scattering operator in the kinetic equation. Diffusion, convection and slowing down are included.
- Critical for RBQ multi-mode cases (Dupree'66, Berk'95, White'18) turns out to be:
  - the resonant frequency and its broadening:
    (V. Duarte APS, AAPPS'20 inv. talks), slide #7 in Zhihong's presentation)

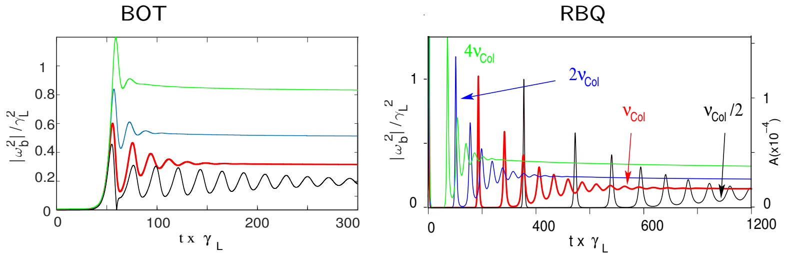
$$res.\ delta\ function\ \delta\left(\Omega=\omega+n\dot{\varphi}-m\dot{\theta}-l\omega_b\right)\rightarrow res.\ window\ function, \mathscr{F}_{l}\left[\Omega\right]$$

RBQ2D computes EP diffusion for the whole device modeling to (1) evolve EP distribution function within TRANSP & (2) evolve it during the run within the code.

Self-consistent diffusion near the resonance region is critical ⇒ New QL theory was developed *(V. Duarte APS'20 inv. talk, PoP paper in preparation).*

RBQ, near threshold wind.funct. & Bump-on-tail (BOT) agree qualitatively (V&V, year 4)

RBQ (Quasi-linear): fixed boundary conditions (BC) on axis, fixed (zero) at the edge.
BOT (fully nonlinear Vlasov kinetic equation solver): Ω, γ_L, γ_d, ν_{eff}, fixed BC at infinity.

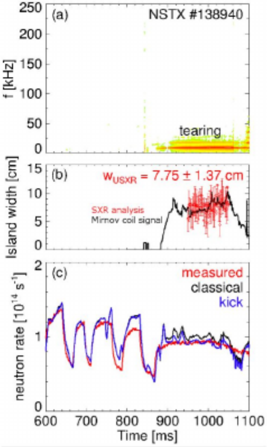


Nominal case for $n=3$, $f=75kHz$: $\gamma_d=-0.75\gamma_L=-2.075\%$ at $\nu_{Coul}=8.9sec^{-1}$ or $\nu_{eff}=8.017\times10^3 sec^{-1}$.

In RBQ the recovery time (repetition rate) scales for nominal DIIID case *(Collins et al., PRL'16)* as $\Delta t(\simeq \nu_{eff}^{-1})=19msec$. In BOT it is $\sim 30msec$ *(Gorelenkov & Duarte, PLA'21).*

Numerical instability may occur in RBQ2D with SUPERLU ADI implementation. Need further studies through ASCR partnership.

Combined NTM & internal kinks in NSTX are addressed with improved kick model



Yang PPCF 2021

- SXR data used to infer island width for 2/1 TM
    - Then rescale Mirnov coil data for time dependent amplitude
- Core kink also detected
- Modes are phase-locked
    - Need to be accounted for in kick model: single transport matrix including effect of both modes
    - Important to obtain neutron rate drop from TRANSP consistent with experiment
- Ongoing: comparison with M3D-C1k (C. Liu)

- Also see D. Liu's work on low-f instabilities in DIII-D

In FY22, 5th year of ISEP SciDAC continue V&V

- V&V for a single, few AEs in DIII-D plasmas, APS'21
- Develop diffusion coefficients interface with NUBEAM, APS'21

  to be used for interfaces with other codes
- Participate in FY2022 OFES Theory Performance Target "Energetic particle confinement properties of ITER operation scenarios will be comprehensively assessed using global gyrokinetic codes, hybrid MHD codes, and reduced EP transport models."

Most critical unresolved issues

- Microturbulence effect on AE saturation:

  selfconsistency to prescribe the microturbulence?

  Zonal Flows / Zonal Structrures / Spectrum ? in near threshold excitation!

- Address microtubrulence with the help from initial value gyrokinetic codes.
- Optimization of most of the codes for GPU computations.
- Study the current drive in the presence of AEs.

I. Publications

1. “Comprehensive magnetohydrodynamic hybrid simulations of fast ion driven instabilities in a Large Helical Device experiment,” Todo, Y.; Seki, R.; Spong, D.A.; Wang, H.; Suzuki, Y.; Yamamoto, S.; Nakajima, N.; Osakabe, M., Physics of Plasmas, 24, n 8, 2017.
2. “Rotation and neoclassical ripple transport in ITER,” Paul, E.J.; Landreman, M.; Poli, F.M.; Spong, D.A.; Smith, H.M.; Dorland, W., Nuclear Fusion, 57, n 11, p 116044 , 2017.
3. “Analysis of Alfven eigenmodes destabilization by energetic particles in TJ-II using a Landau closure model,” Varela, J.; Spong, D.A.; Garcia, L. Nuclear Fusion, 57, n 12, 2017.
4. “Two species drag/diffusion model for energetic particle driven modes,” Aslanyan, V.; Sharapov, S.E.; Spong, D.A.; Porkolab, M. Physics of Plasmas, 24, n 12, p 122511, 2017.
5. “Major results from the first plasma campaign of the Wendelstein 7-X stellarator,” Wolf, RC; Ali, A; Alonso, A; Baldzuhn, J; Beidler, C; Beurskens, M; Biedermann, C; Bosch, HS; ...; Spong, D. A., ...;Zhang, H.; Zhu, J.; Nuclear Fusion 57, 2017.
6. “Overview of the RFX-mod fusion science activity,” Zuin, M.; Dal Bello, S.; Marrelli, L.; Puiatti, M.E.; Agostinetti, P.; Agostini, M.; Antoni, V.; Auriemma, F,… Spong, D. A., …; Nuclear Fusion 57 102012, 2017.
7. V. N. Duarte, H. L. Berk, *et al*, “Theory and observation of the onset of nonlinear structures due to eigenmode destabilization by fast ions in tokamaks”, *Phys. Plasmas* **24**, 122508 (2017). **[selected as both Editor Pick and AIP Scilight]**.
8. V. N. Duarte, H. L. Berk, *et al*, “Prediction of Nonlinear Evolution Character of Energetic-Particle-Driven Instabilities” *Nucl. Fusion* **57** 054001 (2017).
9. M. Podestà et al, Computation of Alfvén eigenmode stability and saturation through a reduced fast ion transport model in the TRANSP tokamak transport code, Plasma Phys. Control. Fusion 59 (2017) 095008

10. *Simulation of toroidicity-induced Alfven eigenmode excited by energetic ions in HL-2A tokamak plasmas*, Hongda He, Junyi Cheng, J. Q. Dong, Wenlu Zhang, Chenxi Zhang, Jinxia Zhu, Ruirui Ma, T. Xie, G. Z. Hao, A. P. Sun, G. Y. Zheng, W. Chen and Z. Lin, *Nuclear Fusion* **58**, 126023 (2018).
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113. Ge Dong, Kyle Gerard Felker, Alexey Svyatkovskiy, William Tang, and Julian Kates-Harbeck. Fully Convolutional Spatio-temporal Models for Representation Learning in Plasma Science. arXiv preprint arXiv:2007.10468, 2020; Journal of Machine Learning for Modeling and Computing, 2(1):49–64 (2021).
114. *Global gyrokinetic simulation with kinetic electron for collisionless damping of zonal flow in stellarator*, Javier H. Nicolau, Gyungjin Choi, Jingyuan Fu, Pengfei Liu, Xishuo Wei, and Zhihong Lin, *Nuclear Fusion* **61**, in press (2021).
115. *Verification and validation of gyrokinetic and kinetic-MHD simulations for internal kink instability in DIII-D tokamak*, G. Brochard, J. Bao, C. Liu, N. Gorelenkov, G. Choi, G. Dong, P. Liu, J. Mc.Clenaghan, J. H. Nicolau, F. Wang, W. H. Wang, X. Wei, W. L. Zhang, W. Heidbrink, J. P. Graves, Z. Lin, H. Lutjens, submitted to *Nuclear Fusion*, 2021.

II. **Invited talks**

1. E.M. Bass, IAEA-FEC oral, 2018.
2. Z. Lin, Transport Task Force Workshop, San Diego, 2018.
3. Z. Lin, DOE SciDAC-4 Principal Investigator Meeting, Washington DC, 2018.
4. Z. Lin, US-Japan JIFT Exascale Computing Workshop, Princeton, 2018.

5. D. A. Spong, “Energetic particle confinement/stability analysis for stellarators and tokamaks,” invited presentation at the 23rd Workshop on MHD Stability Control – A US-Japan Workshop, UCLA, Nov 12 - Nov 16, 2018.
6. D. A. Spong, “Energetic particle physics and optimization methods for stellarators,” US-Japan JIFT Workshop on "Progress on advanced optimization concept and modeling in stellarator-heliotrons", March 22 – 23, 2018, Kyoto University, Kyoto, Japan. (oral-invited).
7. Podestà et al, IAEA-FEC 2018
8. Bardóczi et al, TTF 2018
9. N.N.Gorelenkov et al., TTF 2018 “A Quasi-linear modeling of fast ion relaxation due to Alfvénic instabilities”.
10. N.N.Gorelenkov et al., APS 2018 “Quasi-linear resonance broadened model for fast ion relaxation in the presence of Alfvénic instabilities” invited talk.
11. Z. Lin, 7th Annual Workshop on Fusion Simulation, Wuhan, China, 2019.
12. Z. Lin, 11th International Conference on Computational Physics (ICCP11), Hangzhou, China, 2019.
13. Z. Lin, DOE SciDAC-4 Principal Investigator Meeting, Washington DC, 2019.
14. S. Klasky, 10th International Conference on Computational Methods (ICCM2019), Singapore, 2019.
15. Z. Lin, 61st Annual Meeting of APS Division of Plasma Physics, Mini-Conference on Building Bridge to Exascale Computing: Applications and Opportunities for Plasma Science, Fort Lauderdale, 2019.
16. Z. Lin, US-Japan Compact Torus Workshop (CT2019), Toki, Japan, 2019.
17. Z. Lin, Annual Meeting of Asia-Pacific Physical Society (AAPPS-DPP), Hefei, China, 2019.
18. D. A. Spong, M. Salewski, Simon Pinches, invited oral presentation at ITPA Coordinating Committee Meeting, December 10 – 12, 2019ITPA-Coordinating Committee Meeting “Energetic Particle (EP) Topical Group Report of Activities for 2019.”
19. D. A. Spong, “Interaction of runaway electrons with whistler and Alfvén waves in the presence of impurity injection,” oral presentation at the 7th Annual Theory and Simulation of Disruptions Workshop, Princeton Plasma Physics Laboratory, August 5 - 7, 2019.
20. D. A. Spong, “Energetic Particle Physics Issues for Stellarators and Possibilities for Optimization,” invited oral at the US/Japan Stellarator Workshop, Auburn, Alabama, Feb. 25 – 27, 2019.
21. D. A. Spong, “Energetic Particle (EP) Topical Group Report of Activities for 2018,” invited oral presentation at ITPA Coordinating Committee Meeting 1/1/2019.
22. W. Tang, “Deep Learning Acceleration of Progress Toward Delivery of Fusion Energy, ” Invited Seminar, Microsoft, Corporation Headquarters, Redmond, WA (Nov. 2019);
23. W. Tang, “AI/Deep Learning Acceleration of Progress Toward Delivery of Fusion Energy,” Invited Talk, International Supercomputing Conference (SC’19), Denver, CO (Nov. 2019);
24. W. Tang,"Implementation of an AI-enabled Deep Learning Disruption Predictor into a Tokamak Plasma Control System," Invited Seminar, UC Irvine, Dept. of Physics & Astronomy, Irvine, CA (Dec. 2019).
25. Z. Lin, Annual Meeting of Asia-Pacific Physical Society (AAPPS-DPP) (remote), 2020.
26. C.S. Collins, IAEA-FEC oral, 2020.
27. D. A. Spong, M. Salewski, S. Pinches, invited oral presentation at 2020 ITPA-Coordinating Committee Meeting, December, 2020 “Energetic Particle (EP) Topical Group Report of Activities for 2020.”
28. D. A. Spong, Simons Team Meeting, Virtual Zoom meeting, August 3 – 6, 2020, invited oral presentation “Optimizing stellarators for energetic particle instability suppression/control.”
29. V.N.Duarte “First-principles formulation of resonance broadened quasilinear theory near an instability threshold“, AAPPS, 2020.

30. V.N.Duarte “Integrated two-dimensional quasilinear modeling of fast ion relaxation in tokamaks“, APS invited talk, 2020.
31. W. Tang, “Features of a Possible NSF Roadmap Supporting Science Applications,”, NSF Invitation-Only Smart Cyberinfrastructure Workshop, Crystal City, VA (Feb., 2020);
32. W. Tang “Applications and Techniques for Fast Machine Learning in Science: Plasma Physics/Fusion Energy Science,” Invited Talk, Southern Methodist University, Virtual Conference, Dec., 2020)
33. P. Liu, Transport Task Force Workshop (remote) (plenary), 2021.
34. J. Nicolau, Transport Task Force Workshop (remote) (plenary), 2021.
35. Z. Lin, International Tokamak Physics Activities (ITPA) (remote), 2021
36. Z. Lin, 10th US-PRC Magnetic Fusion Collaboration Workshop (remote), 2021.
37. D. A. Spong, MagNetUS meeting, August 2 – 4, 2021, University of Wisconsin, “Runaway electron driven whistler instabilities in tokamak plasmas.”
38. Yashika Ghai, “Instabilities driven by fast ions in DIII-D plasmas with a negative triangularity,” Transport Task Force Workshop (remote) invited oral talk, 2021.
39. Yang et al, TTF 2021
40. Yang et al, AAPPS 2021
41. Bonofiglo et al, TTF 2021
42. Bonofiglo et al, AAPPS 2021
43. V. Magri, SIAM Conference on Computational Science and Engineering, 2021.
44. G. Dong, ”Advances In Deep-Learning-Based Prediction & Control of Plasma Instabilities and Disruptions in Tokamaks,” Invited Talk, IAEA-PPPL Workshop on Theory and Simulation of Disruptions, July 19-23, 2021.
45. W.Tang, “Deep Learning Acceleration of Progress in Fusion Energy Research,” Invited Seminar, DOE ECP ExaLearn Virtual Meeting, July, 2021

III. **Postdocs**

1. Guillaume Brochard (UCI, 2/2020-present)
2. Gyung Jin Choi (UCI, 5/2019-5/2021)
3. Javier Nicolau (UCI, 4/2019-present)
4. Xishuo Wei (UCI, 2/2019-present)
5. Pengfei Liu (UCI, 1/2019-present)
6. Jian Bao (UCI, 7/2016-12/2018)
7. Lei Shi (UCI, 10/2016-7/2018)
8. Ge Dong (PPPL, 1/2019-present)
9. Bei Wang (PU)
10. Jacobo Varela (ORNL 2017-2018 - now researcher at Universidad Carlos III, Madrid, Spain)
11. Yashika Ghai (ORNL 11/2019-7/2021 - now ORNL theory group member)
12. V.N. Duarte (PPPL 05/2018-09/2020 - now PPPL research stuff)
13. Victor Magri (LLNL, 5/2019-present)
14. Protonu Basu (LBNL, 2017-2018)

IV. **Students**

1. Wenhao Wang (UCI graduate, 2018-present)
2. Sam Taimourzadeh (PhD, UCI, 2018; Employer, Toyota Motor)
3. Calvin Lau (PhD, UCI, 2017; Employer, TAE Technologies Inc.)

4. Matt Leinhauser (University of Delaware graduate student, LBNL summer intern, 2021-present)
5. Kevin Gill (UCI undergraduate, 2021-present)
6. Fukun Yun (UCI undergraduate, 2021-present)
7. Christian Sims (ORNL summer intern 2021 worked with Y. Ghai and D. Spong on gyrofluid closures - Georgia Tech undergraduate)
8. Justin Blanchard (ORISE supported Oak Ridge High School math thesis student worked in 2019 with D. Spong and Diego del-Castillo-Negrete on stochastic particle orbit and magnetic field line maps)