SciDAC ISEP
Integrated Simulation of Energetic Particles in Burning Plamsas

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SciDAC ISEP Center

UCI, GA, PPPL, ORNL, LBNL, LLNL, PU, UCSD, UT

GTC CAAR project

UCI, PU, ORNL, NVIDIA, IBM

Outlines

- ISEP objectives
- ISEP module: first-principle
- ISEP module: reduced models
- ISEP V&V

[D. Pace, W. Heidbrink, M. Van Zeeland, 2015]

SciDAC ISEP: Integrated Simulation of Energetic Particles

- The confinement of energetic particles (EP) is a critical issue for burning plasma experiments since the ignition in ITER relies on the self-heating by energetic fusion products (α-particles)
- Plasma confinement properties in the *new* ignition regime of self-heating by α-particles is one of the most uncertain issues when extrapolating from existing fusion devices to ITER
- **EP turbulence and transport**: EP excite meso-scale instabilities and drive large transport, which can degrades overall plasma confinement and threaten machine integrity
- **Interaction between EP and thermal plasmas**: since EP constitute a significant fraction of plasma energy density in ITER, EP can strongly influence microturbulence responsible for turbulent transport and macroscopic magnetohydrodynamic (MHD) instabilities potentially leading to disruptions
- SciDAC GSEP (2008-2017): new paradigm of nonlinear kinetic simulations of EP turbulence by treating relevant physical processes from micro to macro scales on same footing
- In 2017, GSEP & CSEP (2011-2017) jointly established SciDAC ISEP

ISEP Objectives

- Study EP physics needed for predictive capability using GTC, GYRO, FAR3D, M3D-K
  - EP transport by mesoscale EP turbulence
  - EP coupling with microturbulence and macroscopic MHD modes
- Develop integrated simulation capability for EP physics
  - ISEP framework based on GTC
- Develop EP module with predictive capability for WDM
  - Reduced EP transport models (CGM, RBQ, machine learning)
  - First-principles ISEP framework
- EP module V&V via kick model
- Computational partnership
  - Workflow/data management
  - Solvers
  - Optimization & portability

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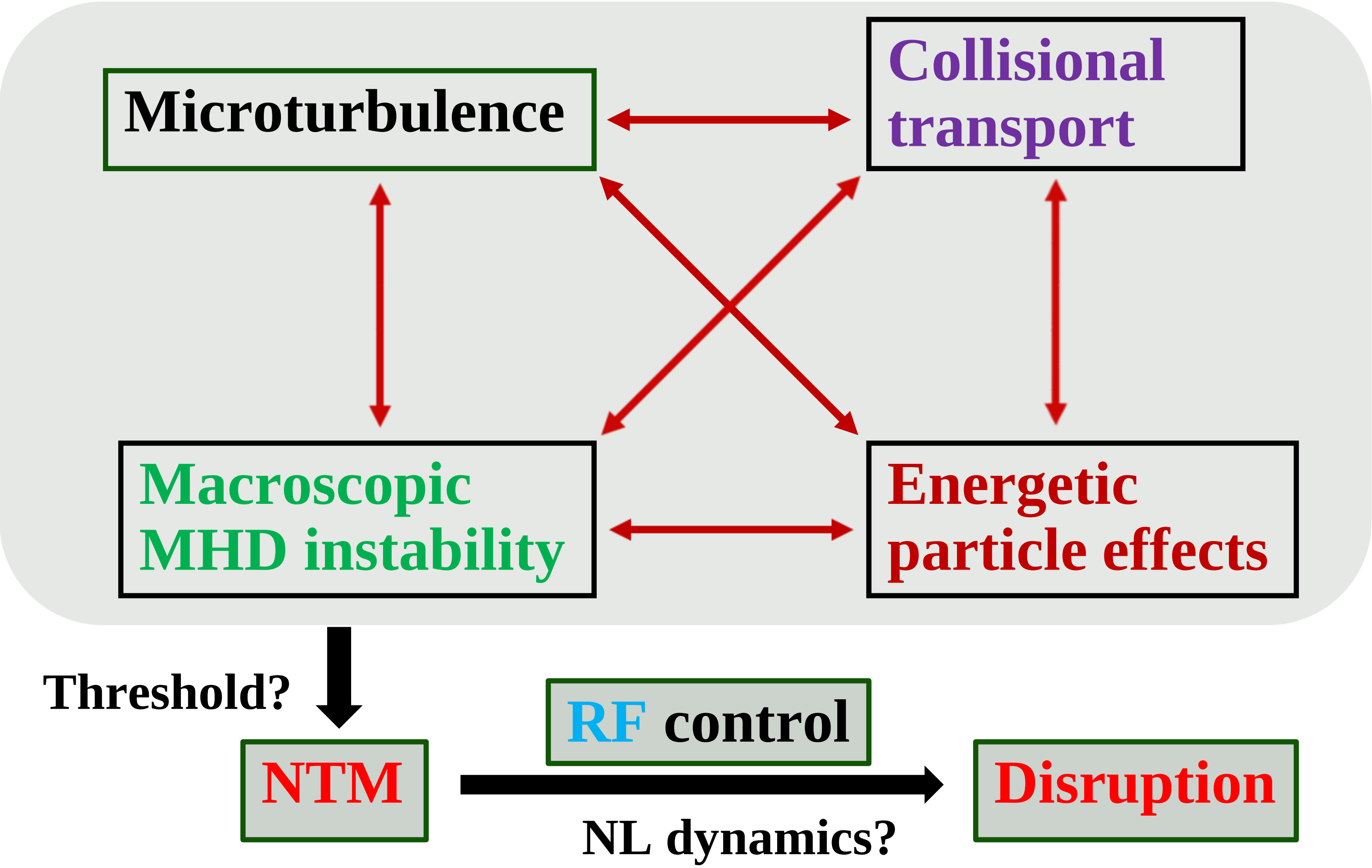
Integrated Simulation Needed to Study Nonlinear Interactions of Multiple Kinetic-MHD Processes



Microturbulence

Collisional transport

Macroscopic MHD instability

Energetic particle effects

Threshold?

NTM

RF control

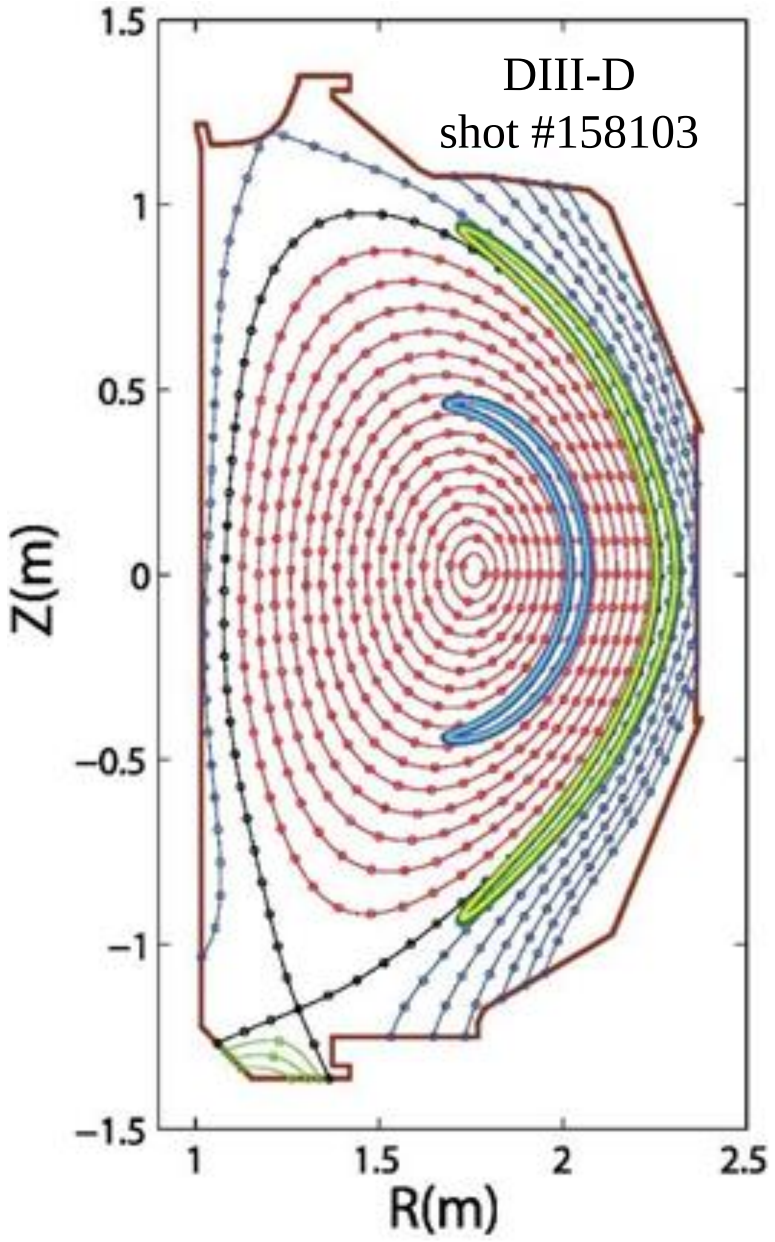
Disruption

NL dynamics?

- Neoclassical tearing mode (NTM) is the most likely instability leading to disruption
- NTM excitation depends on nonlinear interaction of MHD instability, microturbulence, collisional transport, and EP effects. NTM control requires radio frequency (RF) waves

ISEP Framework: First-Principles GTC

- Gyrokinetic toroidal code GTC: PPPL 1993-2002, UCI 2002-
  - ✓ SciDAC GPS (01-11), GSEP (08-17), ISEP (17-)
- First-principles, global, integrated simulation capability for nonlinear interactions of multiple kinetic-MHD processes
- Current capability in the central version
  - ✓ 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



A conservative scheme of drift kinetic electrons for gyrokinetic simulation of kinetic-MHD processes in toroidal plasmas, *J. Bao, D. Liu, Z. Lin, Phys. Plasmas **24**, 102516 (2017)*

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

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

Optimization/Portability for SciDAC-4 ISEP Program

W. Tang & B. Wang (Princeton U.); S. Williams & K. Ibrahim (LBNL)

- **Purpose:** Carry out Performance Optimization and Portability Development in support of SciDAC-4 ISEP via bringing key GTC-P advances achieved to the parent GTC code.

→ Realistic performance analysis of the GTC-P code have been carried out on the KNL system (Stampede II) at the TACC by leveraging Intel's software engineering expertise available through the Intel Parallel Computing Center (IPCC) at Princeton University.

- **Results:** : Substantive progress toward an explicit distribution strategy of the particle and data between MCDRAM and DDR together with efficient performance scaling of GTC-P demonstrated on the large Stampede KNL supercomputing system.

This FY'18 will be completed by Oct. 1, 2018 with the associated software posted on bitbucket[1] by that time.

- **FY'19 Targeted Goals:**

(1) Complete improved optimization of particle routines demonstrated with efficient scaling of GTC-P achieved for the entire KNL Stampede 2 supercomputer – performance optimization example with practical metric of "me to solution." -- thereby contributing valuable "lessons learned" for the parent GTC code; and

(2) Valuable GTC-P performance data collection will be completed using SDE, Advisor, and LIKWID (performance counters) on Cori(KNL) and NVProf on the SummitDev(Pascal GPU). This will require working with NVIDIA to resolve the key obstacle of major slowdown of NVPROF using a counter-based methodology like LIKWID which currently displays no significant slowdown on Cori. Improved understanding of the differences in data movement and flops executed on these two platforms/implementations will also be targeted.

We are partnering with the hypre project in the FASTMath institute to speed up simulation time

R. Falgout,
U. Yang, LLNL

- HYPRE is a highly scalable multigrid linear solvers project
  - Unique user-friendly interfaces.
  - Flexible software design.
  - Used in a variety of applications.
  - Freely available.

hypre high performance preconditioners

R&D 100

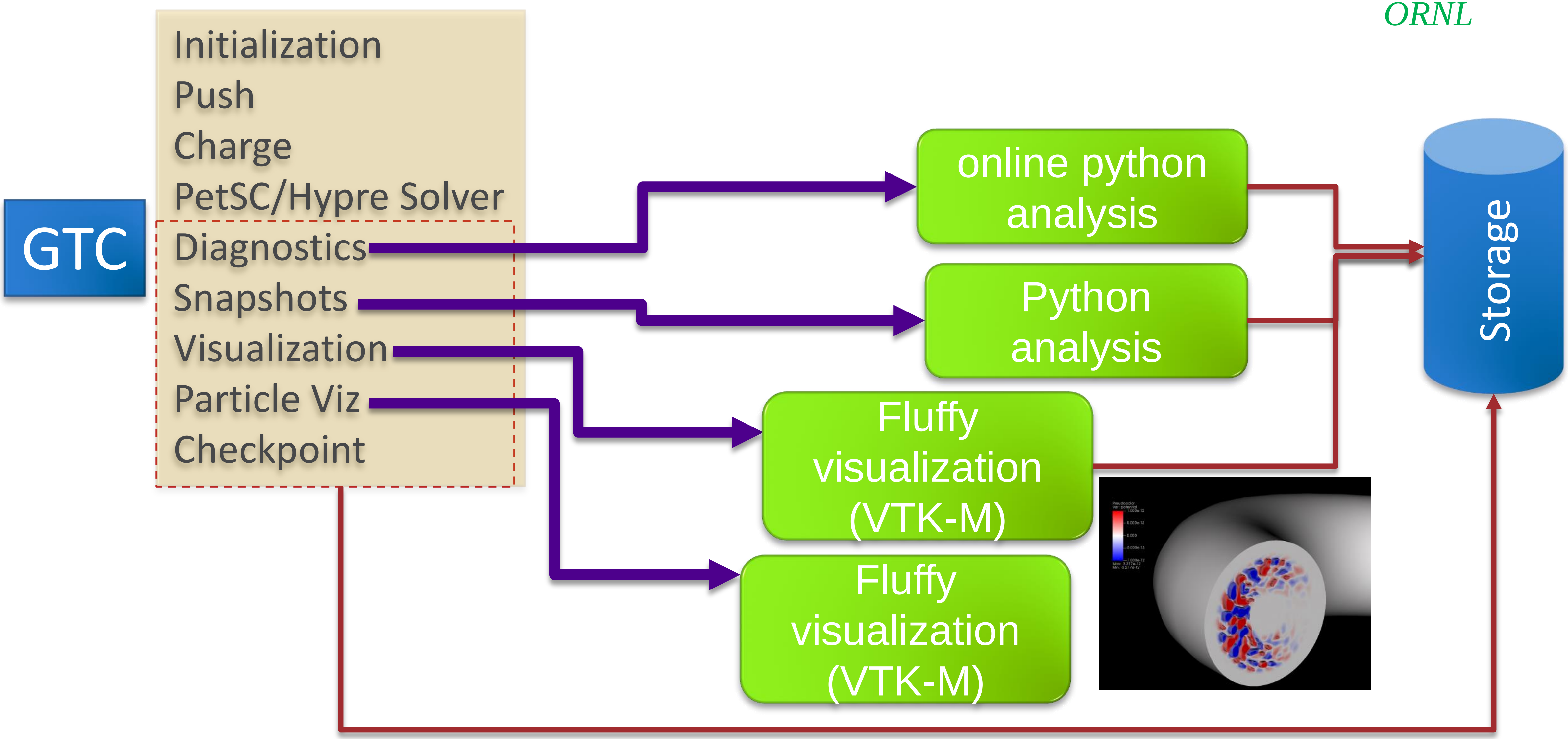
- HYPRE's algebraic multigrid (AMG) solver has already provided significant speedups in GTC using MPI-OpenMP parallelism
  - Field solves can take as much as half the simulation time
  - New work is needed to address new physics, grids, and architectures
  - Minimizing communication and setup costs are key to performance
- Assessing performance and optimizing AMG for current code
- Will also employ new GPU features in hypre and optimize on multi-GPU systems

ISEP Data Management, Visualization, and Analysis

- GTC requires fast I/O for: diagnostics, snapshots (2D analysis), 3D cells(visualization), particles, and checkpoint-restart
- ISEP/RAPIDS implemented ADIOS 2 to achieve this goal
  - Current performance averages over 100 GB/s on Summit
- Python-based analysis routines provided for offline and on-line (in situ) analysis of diagnostics data and snapshot data
- “Fluffy” in situ visualization services for particle and 3D field data are currently being implemented

ISEP Workflow

S. Klasky, ORNL



GTC

Initialization
Push
Charge
PetSC/Hypre Solver
Diagnostics
Snapshots
Visualization
Particle Viz
Checkpoint

online python analysis

Python analysis

Fluffy visualization (VTK-M)

Fluffy visualization (VTK-M)

Storage

ADIOS engines: Synchronous C/R, Synchronous connection to ASCENT, Asynchronous connection to Fluffy-VTK-M, Synchronous Writes for Analysis

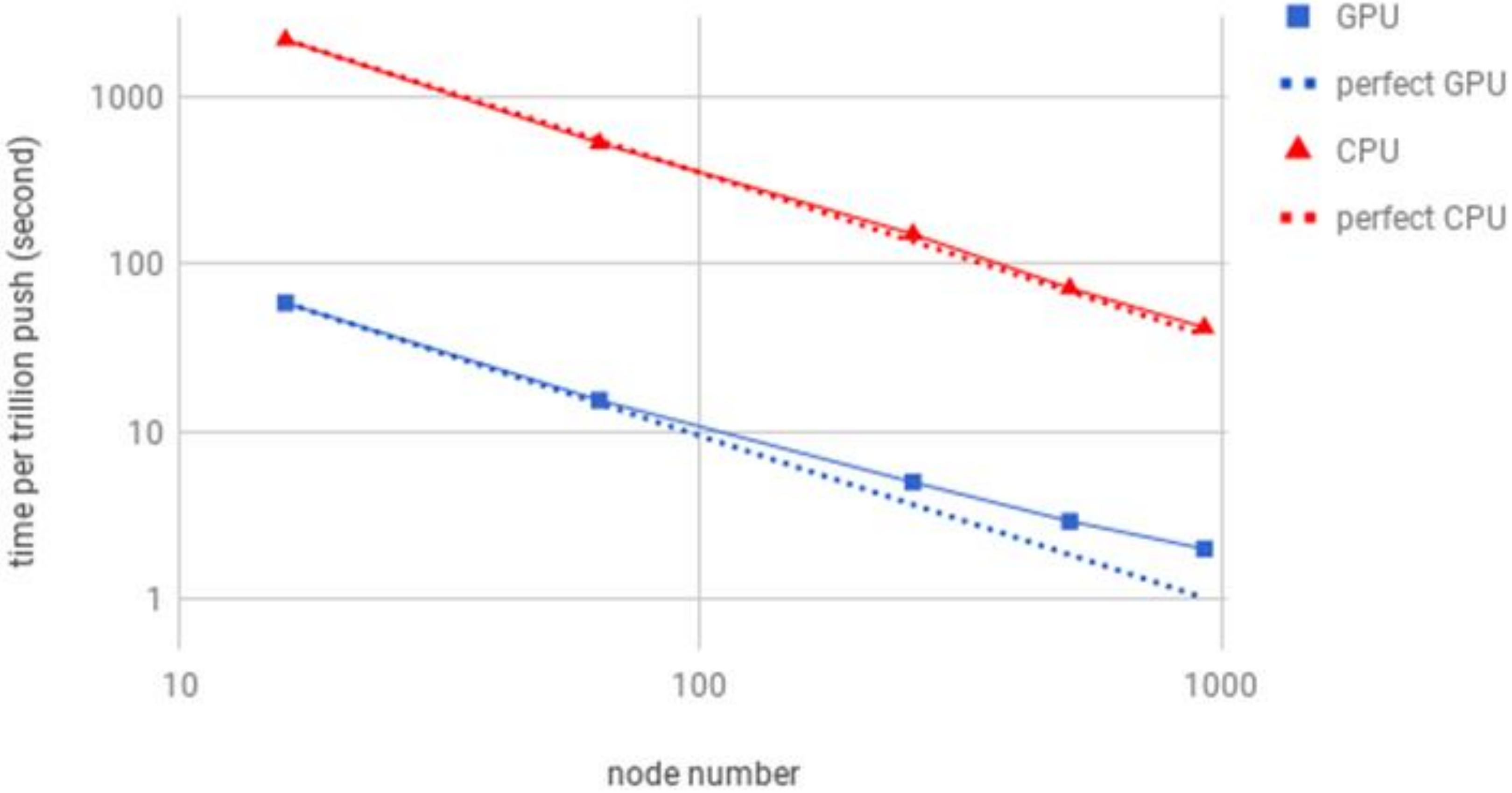
GTC Optimization on Summit GPU

- Use MPI-OpenMP for CPU and one MPI process per GPU
- Use OpenACC and CUDA on GPU
- Move all computing-intensive particle and field data to GPU
- Group MPI toroidal communicator, not particle communicator, to speed up shifting particles
- Particle radial binning to improve data locality
- OpenACC atomic directive for scattering operations
- Enable texture cache for gather operations
- Optimize local memory access and data structure of large array
- Use NVidia GPU sparse linear solver *AmgX*

GTC CAAR team: P. Wang (NVIDIA), W. Joubert (ORNL),
M. Niemerg (IBM), B. Wang, W. Tang (PU), W. Zhang,
S. Taimourzadeh, C. Lau, L. Shi, J. Bao, Z. Lin (UCI)

GTC Performance on Summit GPU

- 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)
- Recently selected by *NVIDIA* as Top 15 App Worldwide
- Ported to Tianhe-3 prototype



Wall-clock time for one trillion particle pushes in GTC weak scaling test on Summit

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Resonance Broadened QL model is developed in 1D version: RBQ1D (N.N.Gorelenkov, V. Duarte, PPPL)

[N. Gorelenkov, Poster]

- DF follows Vlasov kinetic equatioin: Berk, Breizman at al. NF'95,96:

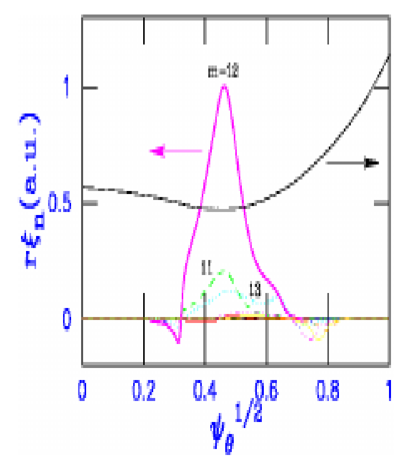
$$\frac{\partial f}{\partial t} = \pi \sum_{l,M} \frac{\partial}{\partial P_\varphi} C_M^2 \mathscr{F}_{lM} \frac{\partial}{\partial P_\varphi} f_{lM} + \nu_{\mathrm{eff}}^3 \sum_{l,M} \frac{\partial^2}{\partial P_\varphi^2} \left(f_{lM} - f_0\right),$$

- Alfvenic Eigenmodes satisfy amplitude evolution equation:

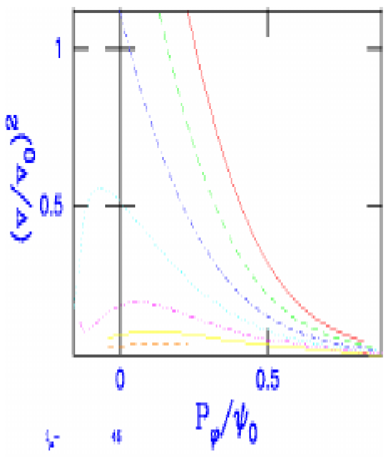
$$C_M(t) \sim e^{(\gamma_L-\gamma_d)t} \Rightarrow \frac{dC_M^2}{dt} = 2\left(\gamma_L-\gamma_d\right) C_M^2$$

2018 APS invited & IAEA oral

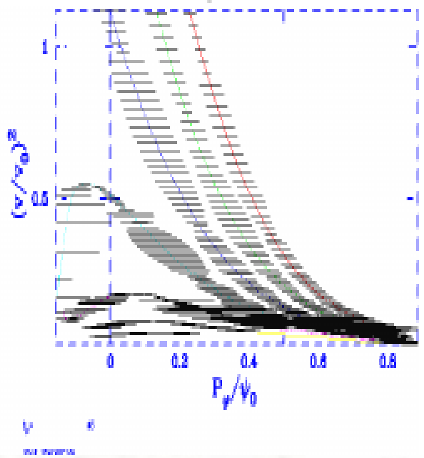
Structure from NOVA

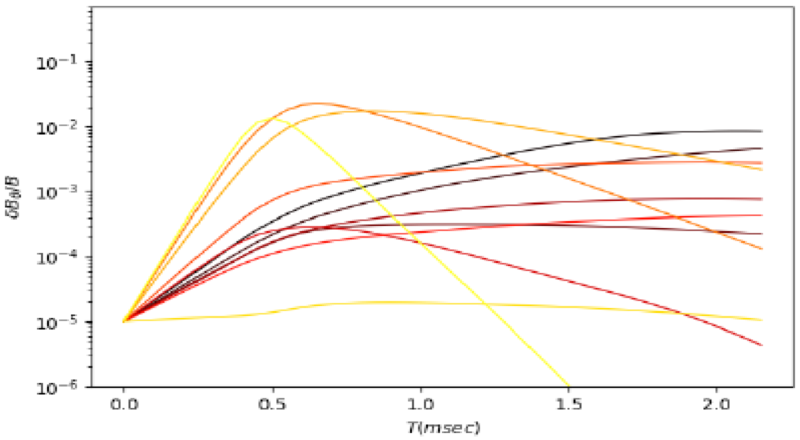


Resonances from NOVA-K



Broadening from RBQ





RBQ finds evolution amplitude of 11 AE modes in DIIID shots

ALPHA is a 1D EP critical-gradient transport model with a fusion/beam source and collisional sink

Alpha transport model

$$\frac{\partial n_{EP}}{\partial t} = S\left(1 - \frac{n_{EP}}{n_{EP0}}\right) - \nabla\cdot\Gamma_{EP} \rightarrow 0$$

fusion or beam source

slowing-down sink

Diffusive EP flux:

$$\Gamma_{EP} = -\left(D_{\mathrm{micro}} + D_{\mathrm{AE}}\right)\nabla_r n_{EP}$$

D_{micro} is the estimated effective background diffusion coefficient from the Angioni model[1] and **known power flux** (therefore known χ_{eff}).

Critical gradient as a function of r determined externally, the **crucial input**.

Boundary condition: Edge n_α is set to zero (pessimistic edge loss estimate).

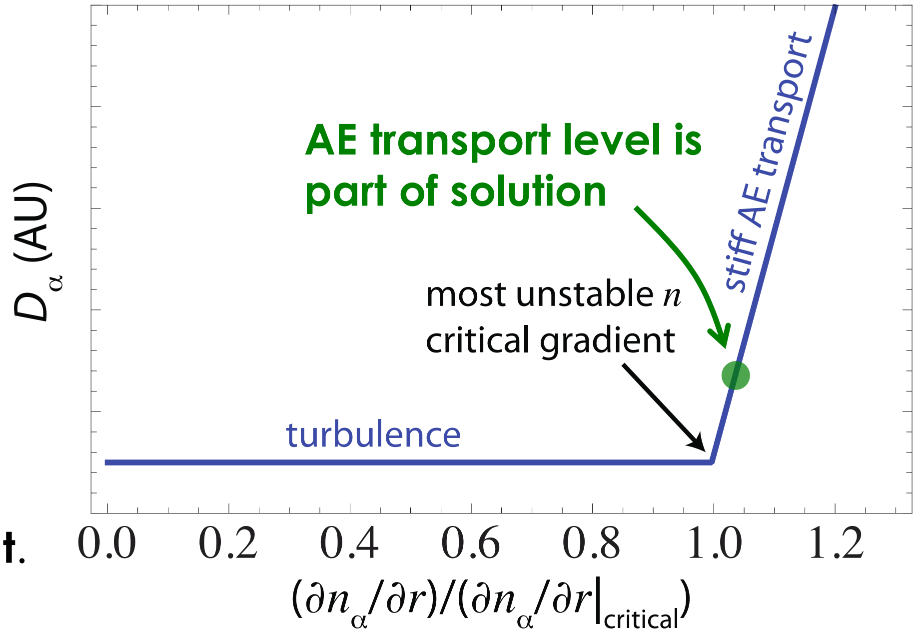
[R. Waltz & E. Bass 2018 IAEA oral]

$$S = n_{\mathrm{D}} n_{\mathrm{T}} \langle \sigma \mathrm{v} \rangle_{\mathrm{DT}}$$

fusion source

$$n_{EP0} = \int_0^\infty \frac{S\tau_s}{2} \frac{\Theta(\mathrm{E}_\alpha - \mathrm{E})}{\mathrm{E}_c^{3/2} + \mathrm{E}^{3/2}} \mathrm{E}^{1/2} d\mathrm{E}$$

Gaffey 1976



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[1] Angioni and Peters, PoP **15** 052307 (2008)

Big Data ML/DL Connection to SciDAC-4 ISEP

W. Tang, PU

- **Fusion Energy Mission**: -- *Most critical problem for tokamaks/ITER is to avoid/mitigate large-scale major disruptions.*
- **Machine Learning Connection to FES HPC Discovery Science:**
  -- ***Rapid Advances*** *now demonstrated of predictive methods via large-data-driven* ***"machinelearning/deep learning" statistical methods***
  -- *Key Approach: Deep Learning Convolutional and Recurrent Neural Nets*
  -- *Significance:* *Demonstrably faster and more accurate predictive alternative to main-line "hypothesis-driven/first principles" path-to-exascale predictive methods.*
  -- *COMPLEMENTARITY/CONVERGENCE of ML & HPC: Exascale HPC can develop DL Classifiers from reduced-models emerging from path-to-exascale simulations of key burning plasma/EP physics such as NTM's – (also a key SciDAC-4 ISEP target!).*
- **Associated Challenge:**
  → *Need to achieve > 95% success rate, <5% false positives at least 30 ms before disruptions*
  -- *with portability of software to ITER via enhanced physics fidelity (capturing multi-D) with improvement in execution time enabled by access to advanced HPC hardware (e.g., large GPU systems such as SUMMIT.*

NOTE: Recently achieved DL capability to move from only scalar ("zero-D") signals to 1D and possibly higher-D can realistically enable incorporating reduced-model NTM classifiers.

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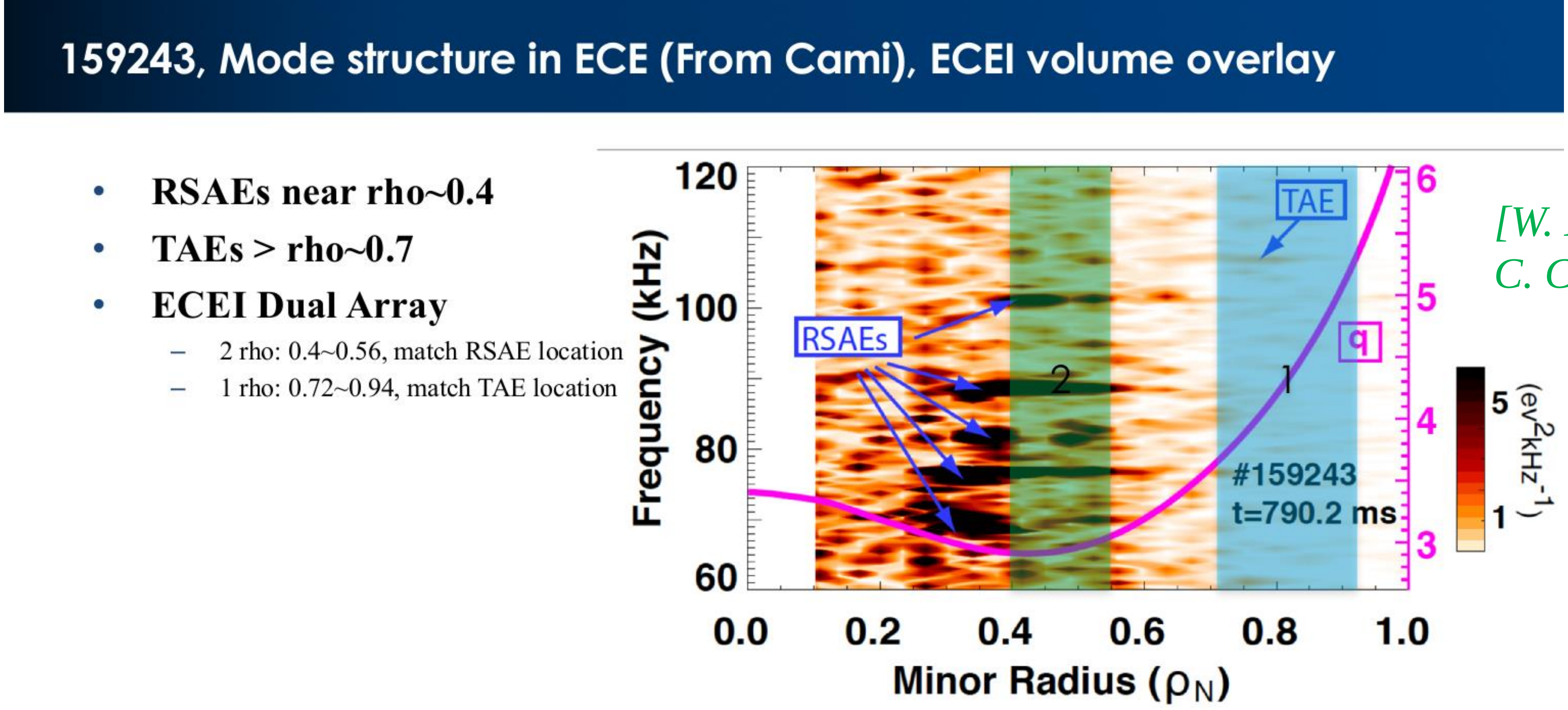


159243, Mode structure in ECE (From Cami), ECEI volume overlay

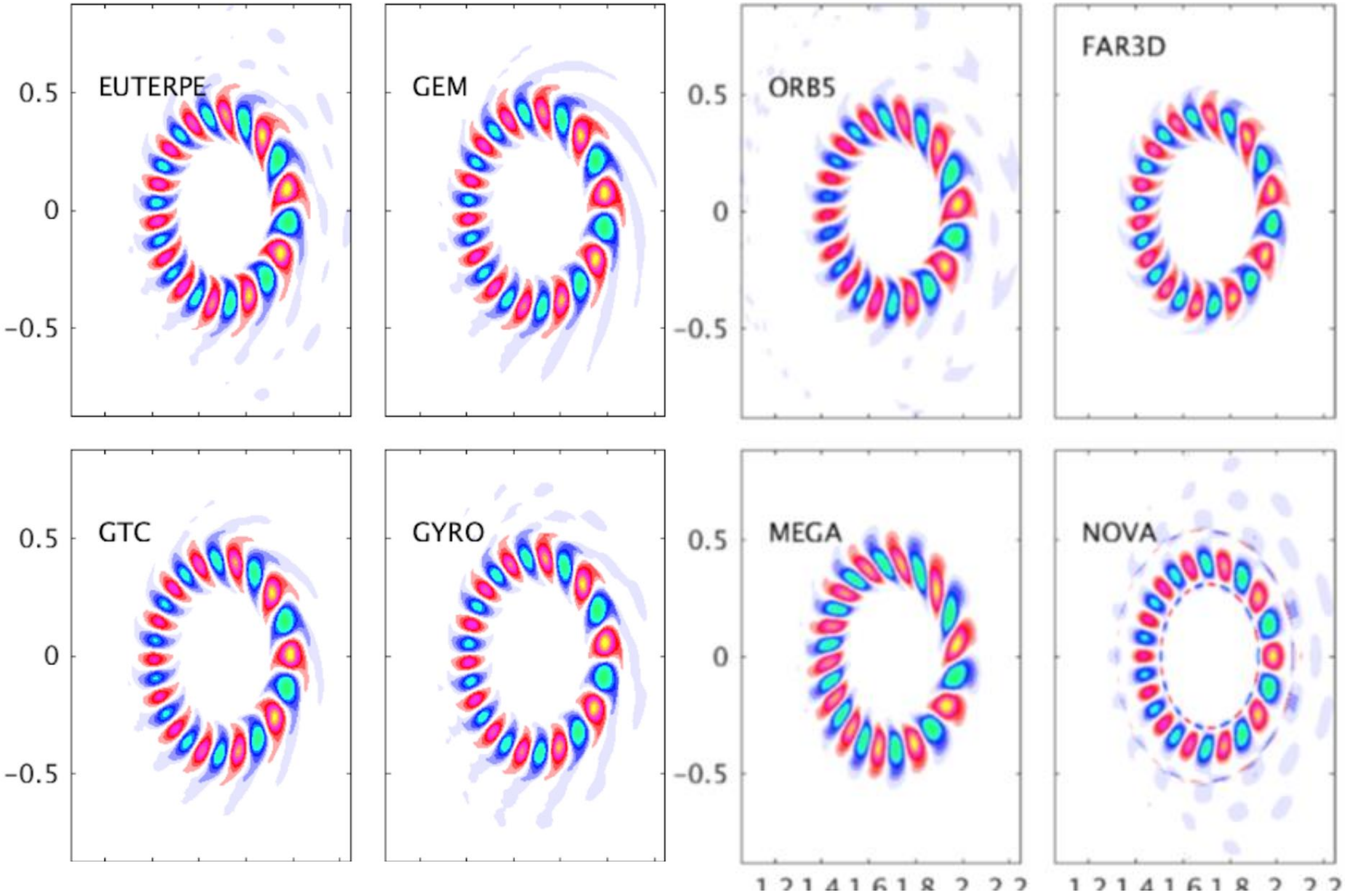
- **RSAEs near rho~0.4**
- **TAEs > rho~0.7**
- **ECEI Dual Array**
  - 2 rho: 0.4~0.56, match RSAE location
  - 1 rho: 0.72~0.94, match TAE location

[W. Heidbrink, C. Collins, 2016]

- RSAE, RSAE, microturbulence co-exist
- What is saturation & transport mechanisms?
- Linear & nonlinear V&V of 8 GK & MHD simulation of RSAE/TAE
- V&V of 3 reduced EP transport models
- Linear benchmark nearly done. Nonlinear simulation in progress

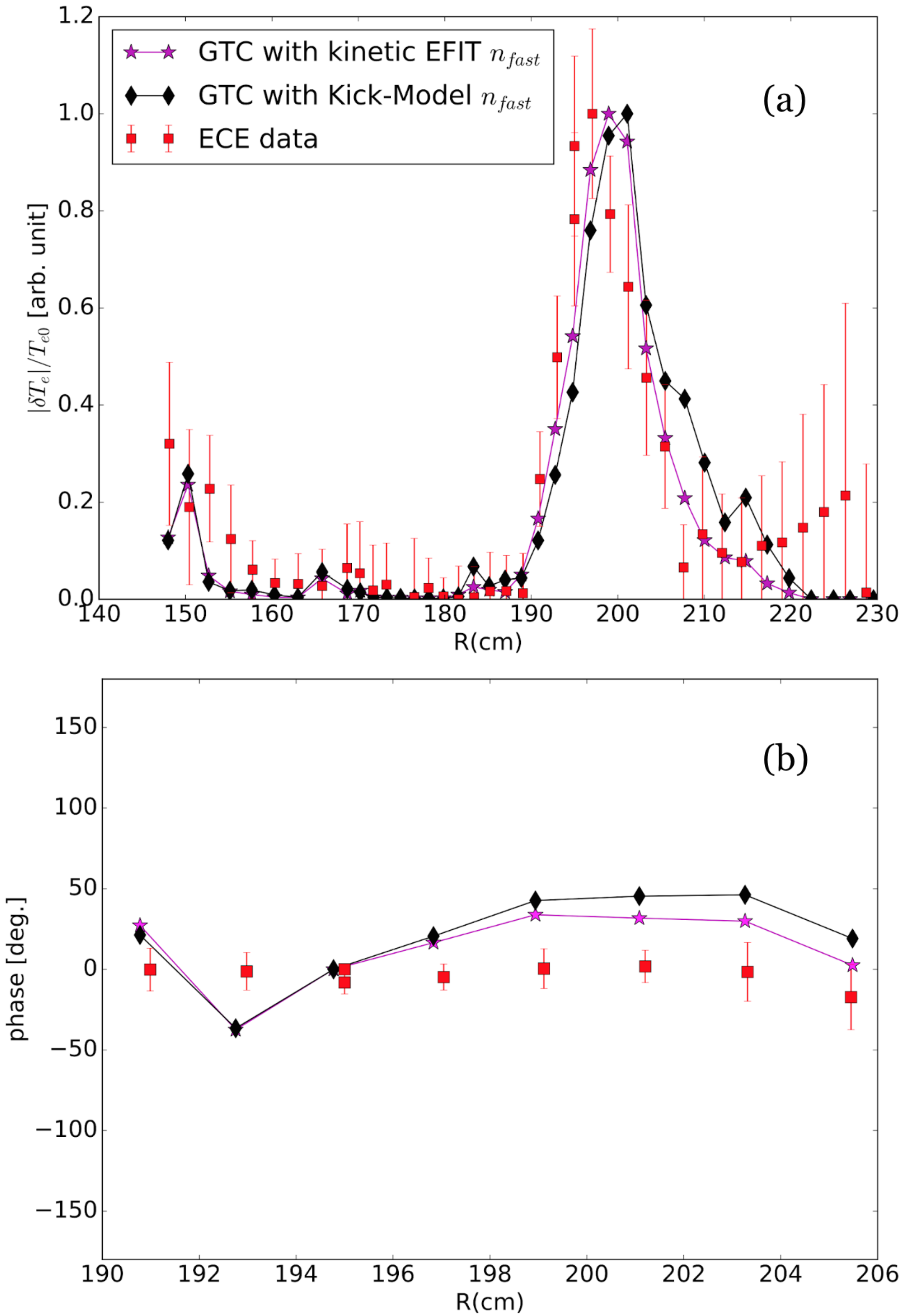
n=4 RSAE in DIII-D shot 158243 at 805ms

[D. Spong, Poster; ITPA EP]



Validation via Synthetic Diagnostics

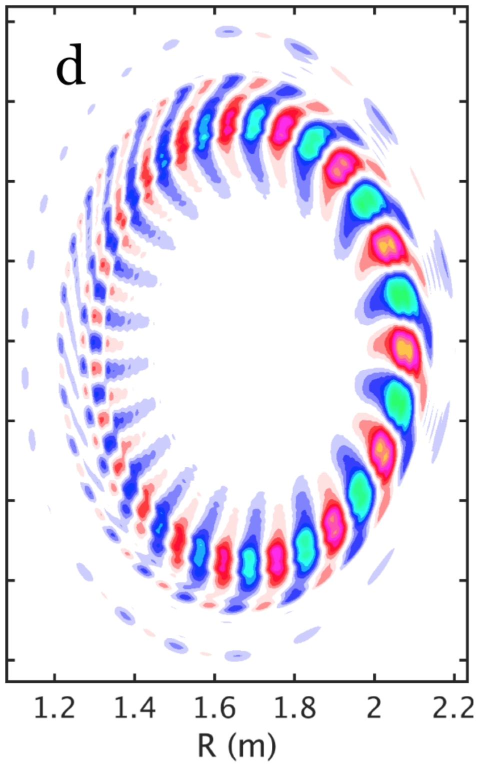
Comparison of GTC simulation with experimental ECE data using Synthetic Diagnostic Platform *[L. Shi et al, 2017]*. (a) Radial structure of δT_e of n = 4 mode. (b) Mode phase with respect to R = 195.0 cm.

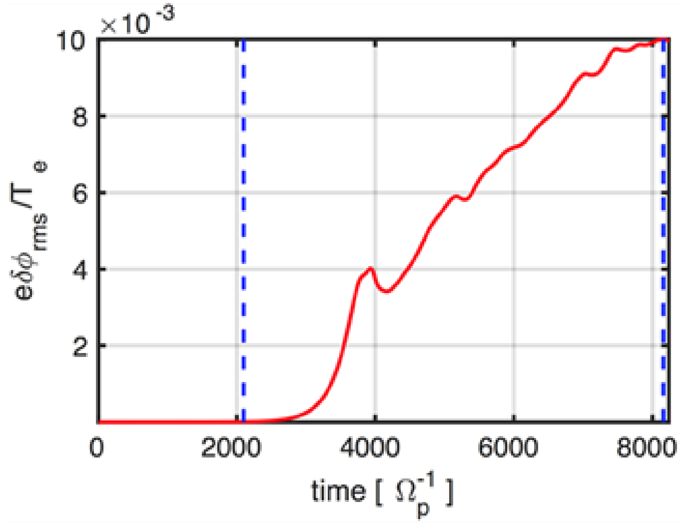


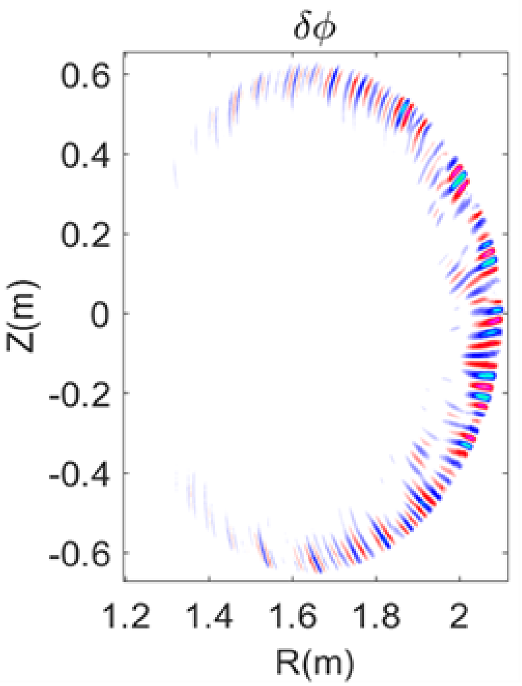
[S. Taimourzadeh
L. Shi, W. Heidbrink,
M. Podesta et al, 2018]

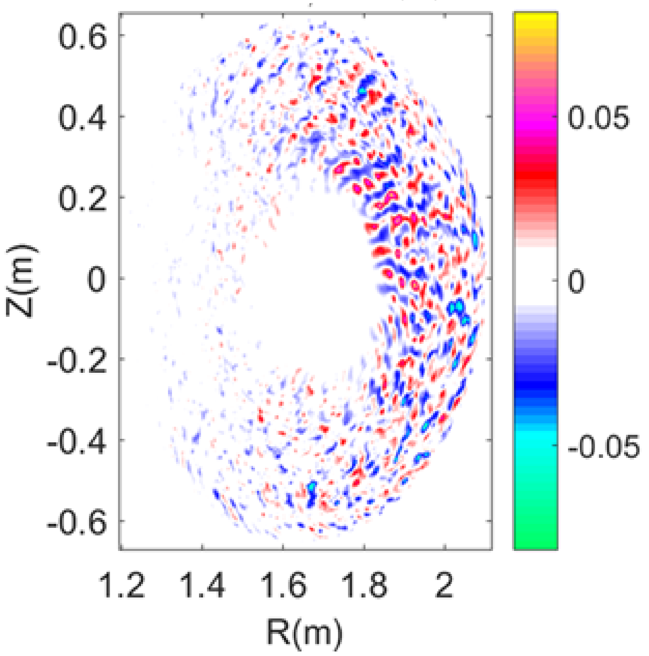
Nonlinear Interaction of RSAE, TAE, ITG

- Using EP profile from kick model, GTC finds n=6 TAE weakly unstable in the outer edge, good agreement with DIII-D
- GTC finds strong ITG instability in the outer edge, nonlinearly spreading to core



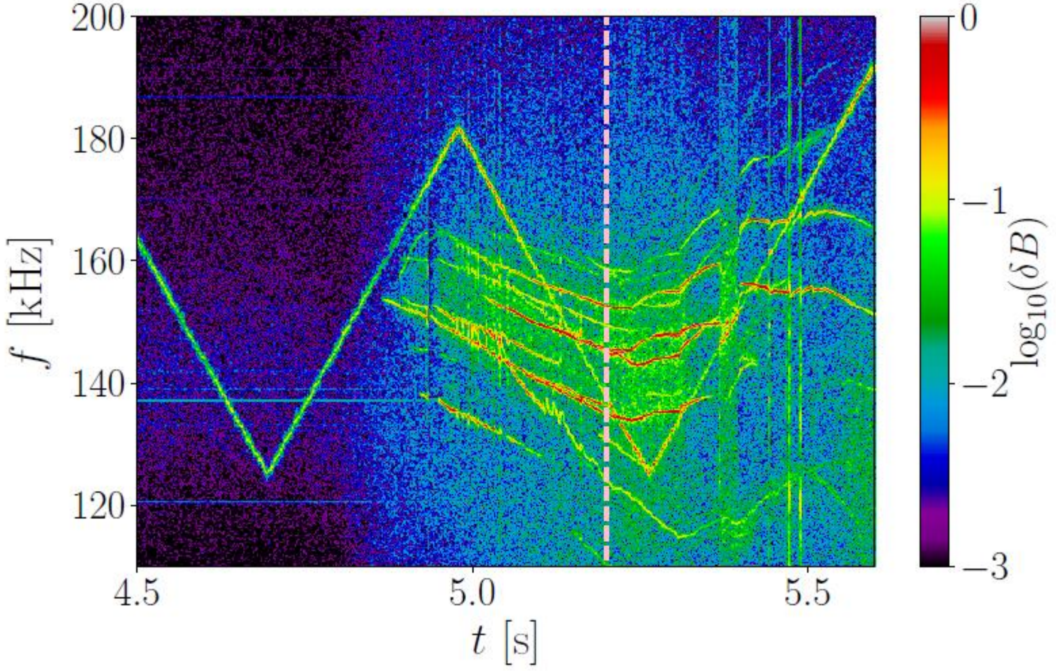


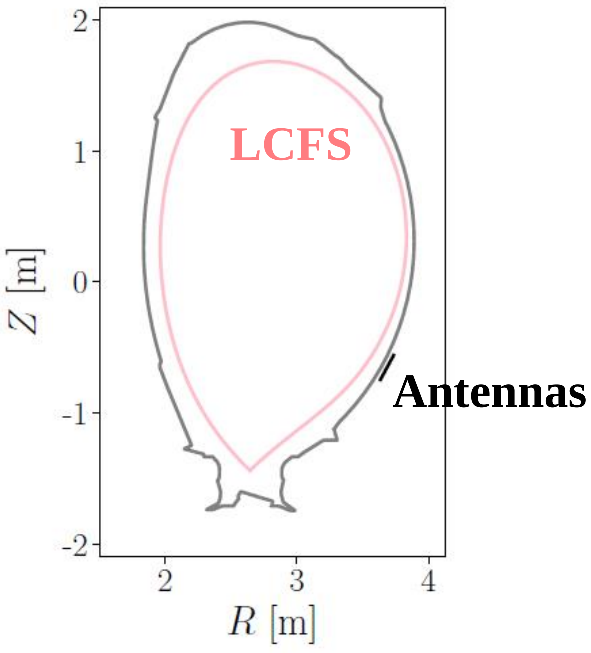




[R. He, 2018]

Recent TAE experiments on JET



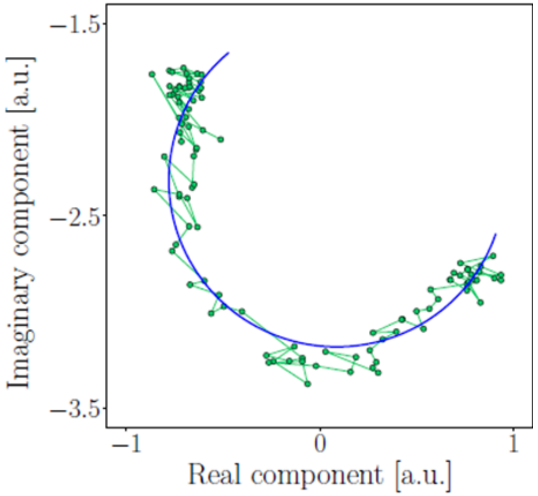


*[V. Aslanyan,
N. Fill,
M. Porkolab,
GTC team,
2018]*

- **TAEs destabilized in presence of NBI and ICRH**
- **External antenna array used to probe marginally stable TAEs**
- **Scenarios to be repeated during DT experiments to observe purely fusion alpha driven TAEs**

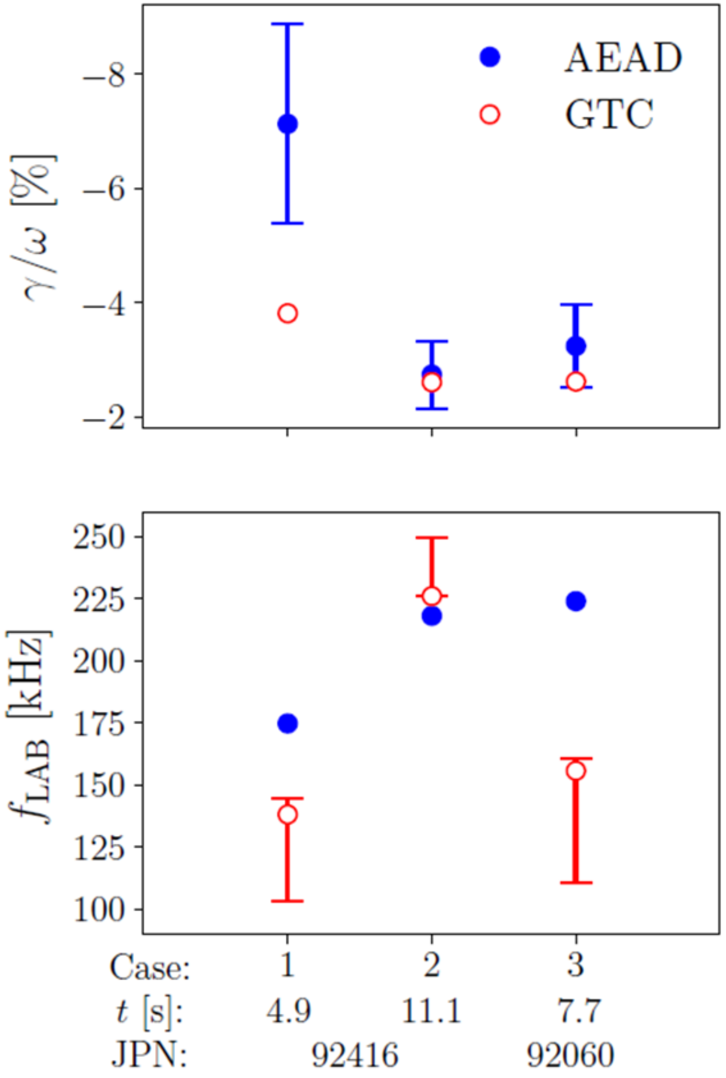
Antenna measurements

- **Three measurements of marginally stable TAEs made in two discharges by the Alfvén Eigenmode Active Diagnostic (AEAD)**
- **Frequency and damping rate deduced from transfer function:**



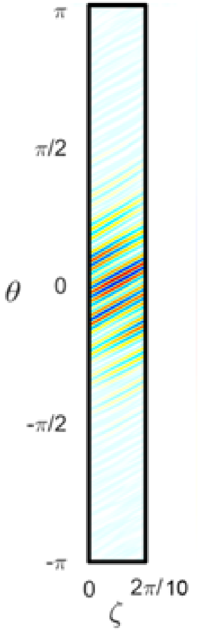
$$H(\omega_d) = \frac{C\omega^2 + iD\omega_d\omega}{\omega^2 - \omega_d^2 + 2i|\gamma|\omega_d}$$

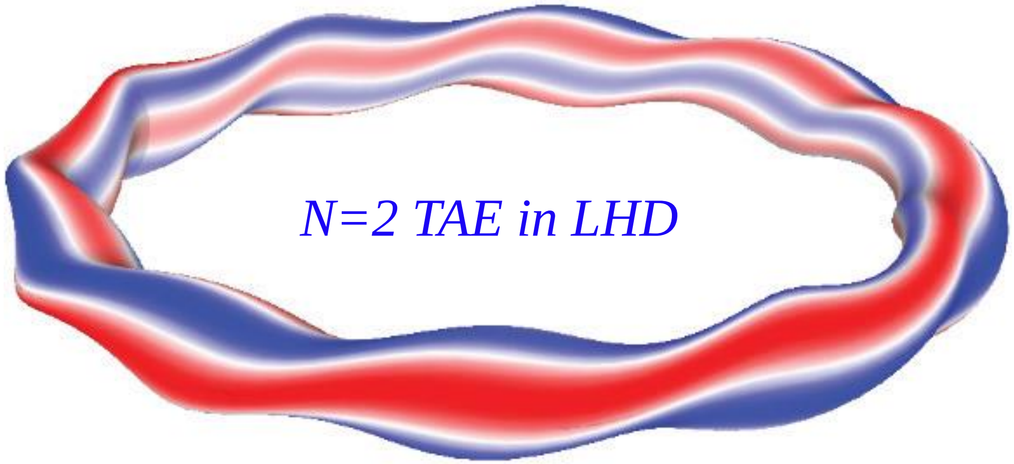
- **Error bars in damping rate measurement arise from uncertainty in the transfer function fits**
- **Difficult to account for high plasma rotation (which has high experimental uncertainty) in cases 1, 3**



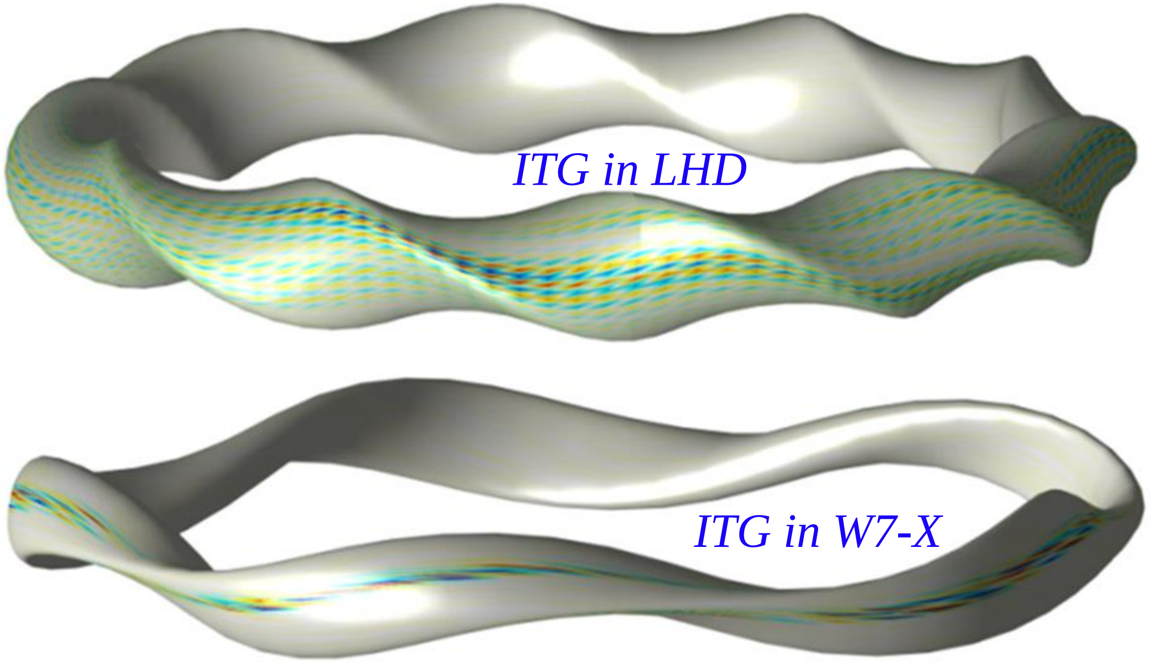
ISEP Framework Simulations of LHD & W7-X Stellarators

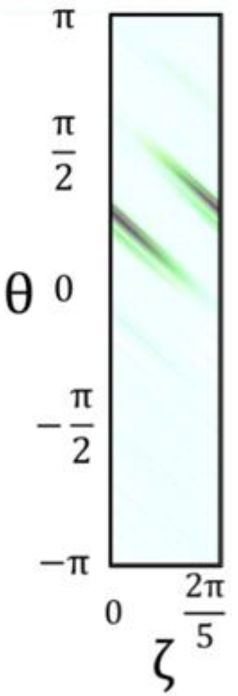
- What are the properties of turbulent transport and energetic particle confinement in stellarators optimized for neoclassical transport?
- GTC linear simulations of toroidal Alfven eigenmode (TAE) in LHD carried out
- GTC growth rate & frequency of ion temperature gradient (ITG) instability agree with EUTERPE; Mode structure in W7-X localized, LHD extended in toroidal direction





*[D. Spong et al, Nuclear Fusion **57**, 086018 (2017)]*



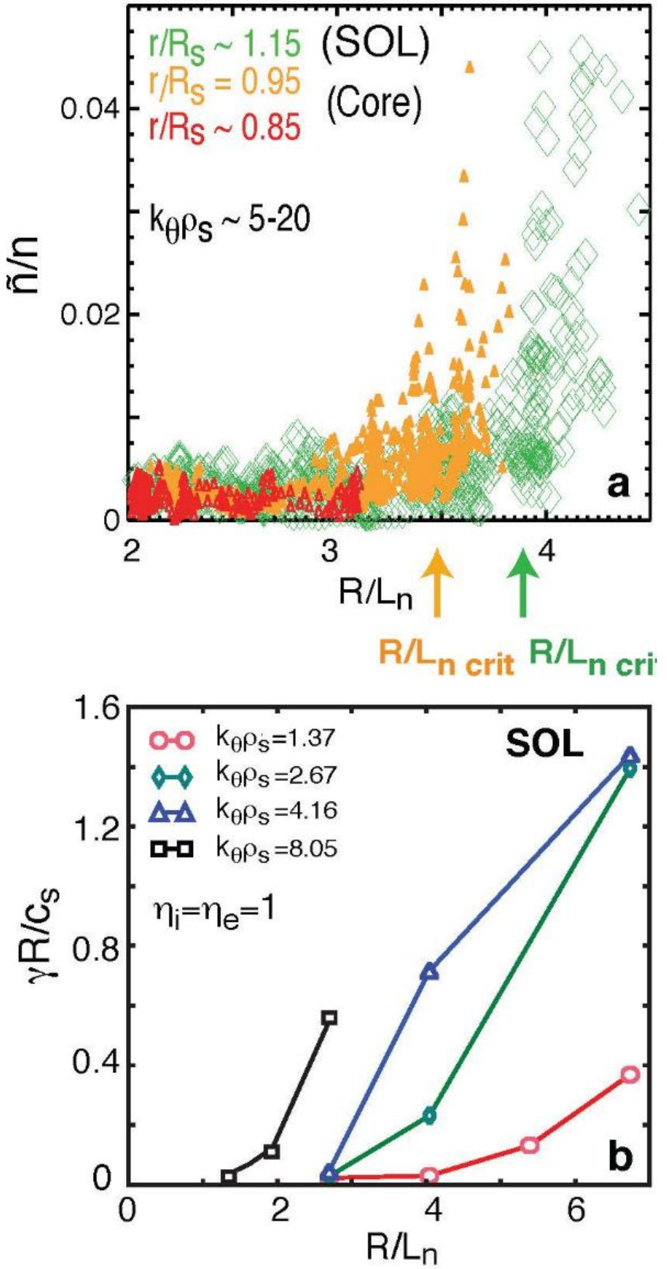


[H. Wang, J. Riemann et al, 2018]

ISEP Framework Simulations of Field Reversed Configuration

- FRC emerged as promising alternate for compact fusion reactor
  - ✓ Macroscopic stability control of C-2 FRC @ TAE Technology *Inc*
- Can FRC be heated and sustained at fusion-relevant regime ($nT\tau$)?
- Microscopic driftwave expected unstable in FRC due to bad curvature, but GTC finds ion-scale modes stable in FRC core
  - ✓ Stabilized by magnetic gradient, large Larmor radius, short field lines
- GTC finds SOL driftwaves unstable with critical pressure gradient, agree with C-2 FRC; SOL turbulence spreads into core
- Fruitful public-private partnership
  - ✓ Trained UCI graduate students for research team at TAE Technology Inc.
  - ✓ Initial development of TAE turbulence simulation code ANC

Suppressed ion-scale turbulence in a hot high-β plasma, L. Schmitz, D. P. Fulton, E. Ruskov, C. Lau, B. H. Deng, T. Tajima, M. W. Binderbauer, I. Holod, Z. Lin, H. Gota, M. Tuszewski, S. A. Dettrick, L.C. Steinhauer, Nature Communications ***7****, 13860 (2016)*



SciDAC ISEP: Integrated Simulation of Energetic Particles

- **First principles ISEP framework and reduced transport model being developed as EP modules in fusion whole device modeling (WDM)**
- **Collaborations with RAPIDS/FASTMath and CAAR project enable ISEP framework to fully utilize pre-exascale computing resources for new physics discovery**
- **ISEP leading EP V&V in world fusion program**
- **Possible integration**
  - ► **Integrate ISEP reduced EP transport models (CGM, RBQ, Kick) in fusion WDM**
  - ► **Integrate physics models in first-principles ISEP framework (GTC) simulation of neoclassical tearing mode (NTM) threshold**
  - ► **Couple machine learning with physics-based EP models?**