Decadal Assessment of Plasma Physics: Perspectives on Computational Plasma Physics

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

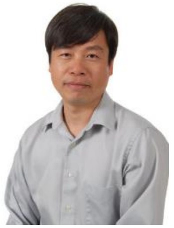
Plasma Physics at UCI

Experiment, Theory & Simulation

Chris Barty

Franklin Dollar

William Heidbrink



Zhihong Lin

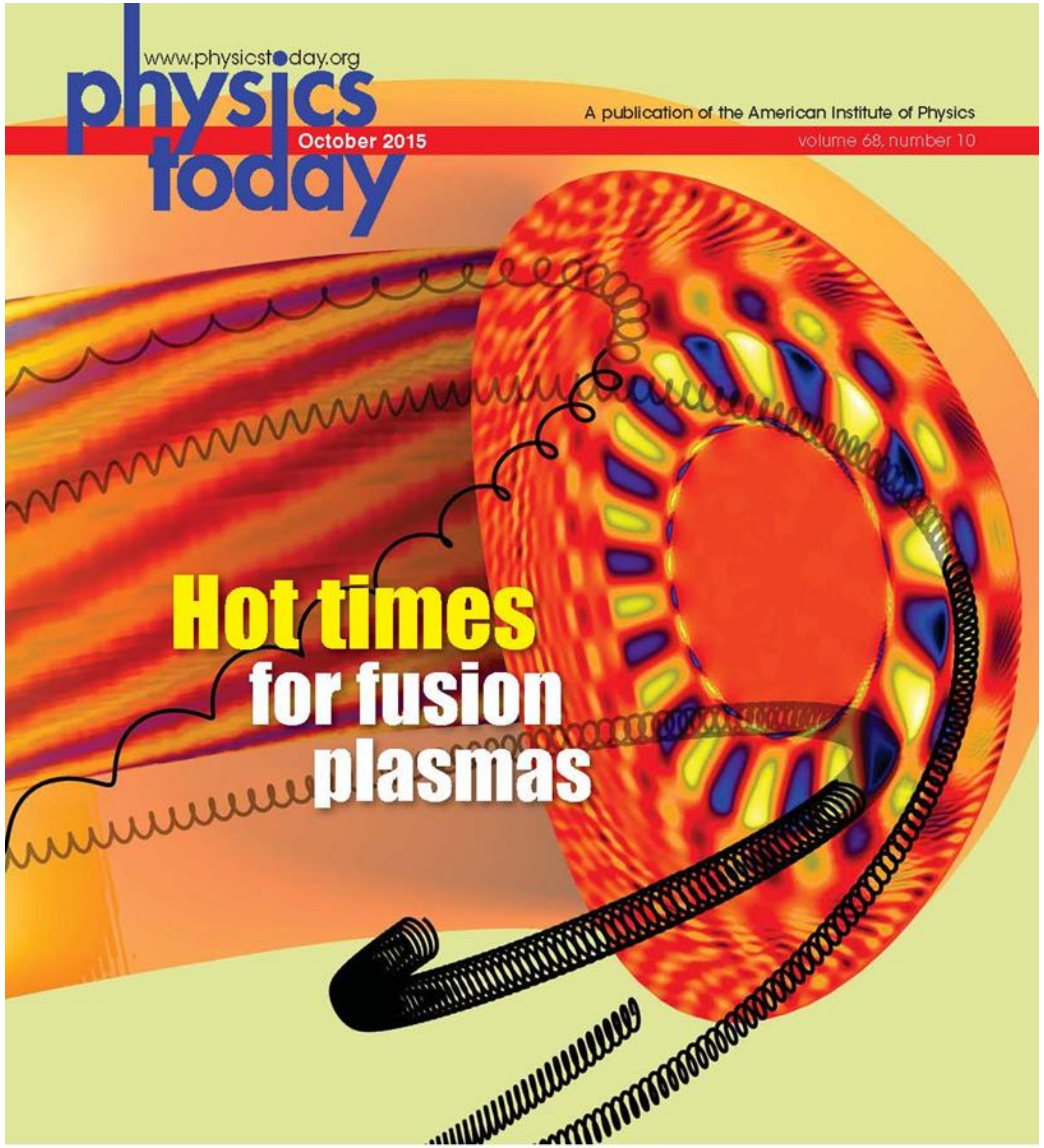
Roger Mcwilliams

Toshiki Tajima
APS Wilson Prize 2019
EPS Alfven Prize 2019
AAPPS Chandraskhar Prize 2018

Liu Chen, *Emeritus*
APS Maxwell Prize 2012
EPS Alfven Prize 2008

Outlines

- Integrated fusion simulation requires coordinated program
- Case study: SciDAC ISEP
- International collaborations
- Public-Private partnership



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

Integrated Simulation Needed to Fill Physics Gap in Whole Device Modeling

- Whole device modeling (WDM): full discharge modeling, mostly reduced models, loosely coupled codes (modules), validity of extrapolation to new regime of burning plasmas?
- Integrated simulation: first-principles simulation of multiple physical processes to provide a WDM module for critical physics, more efficient in a multi-physics code

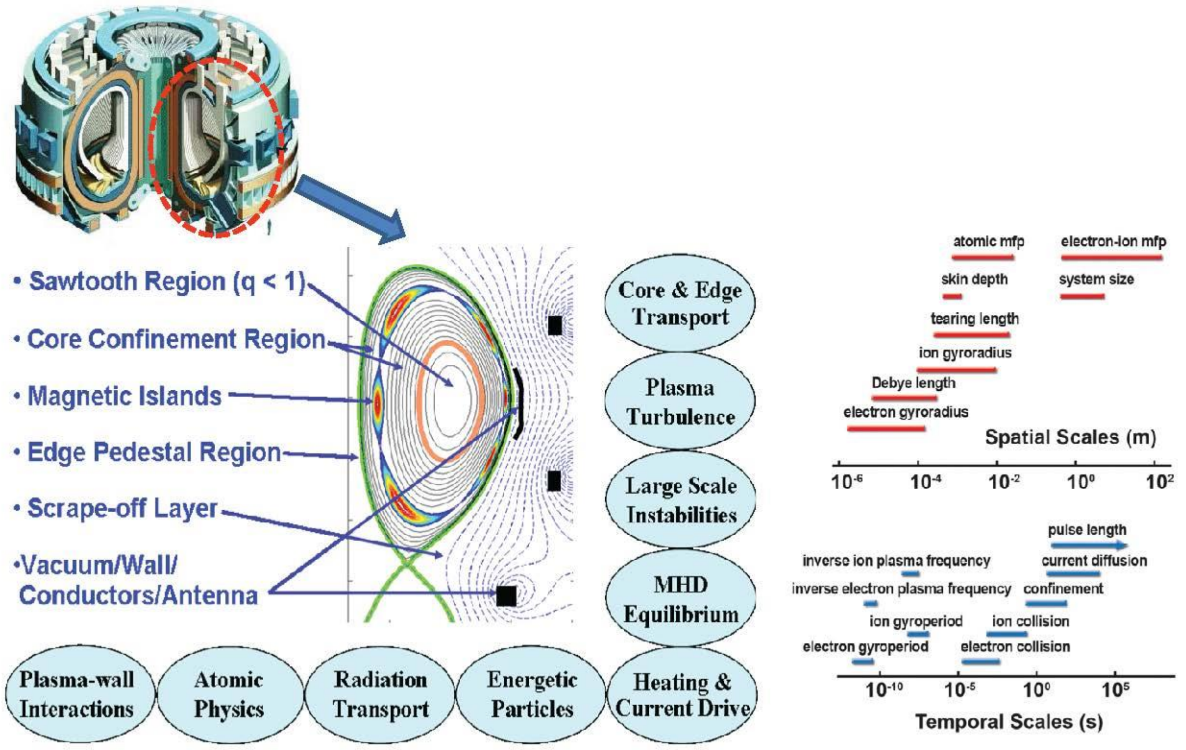
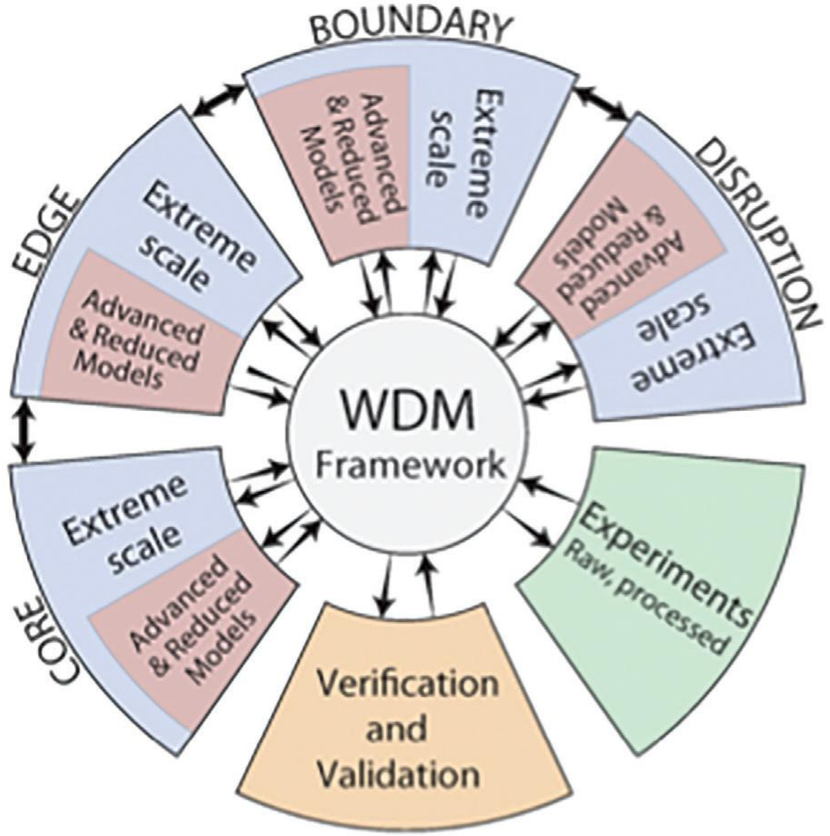


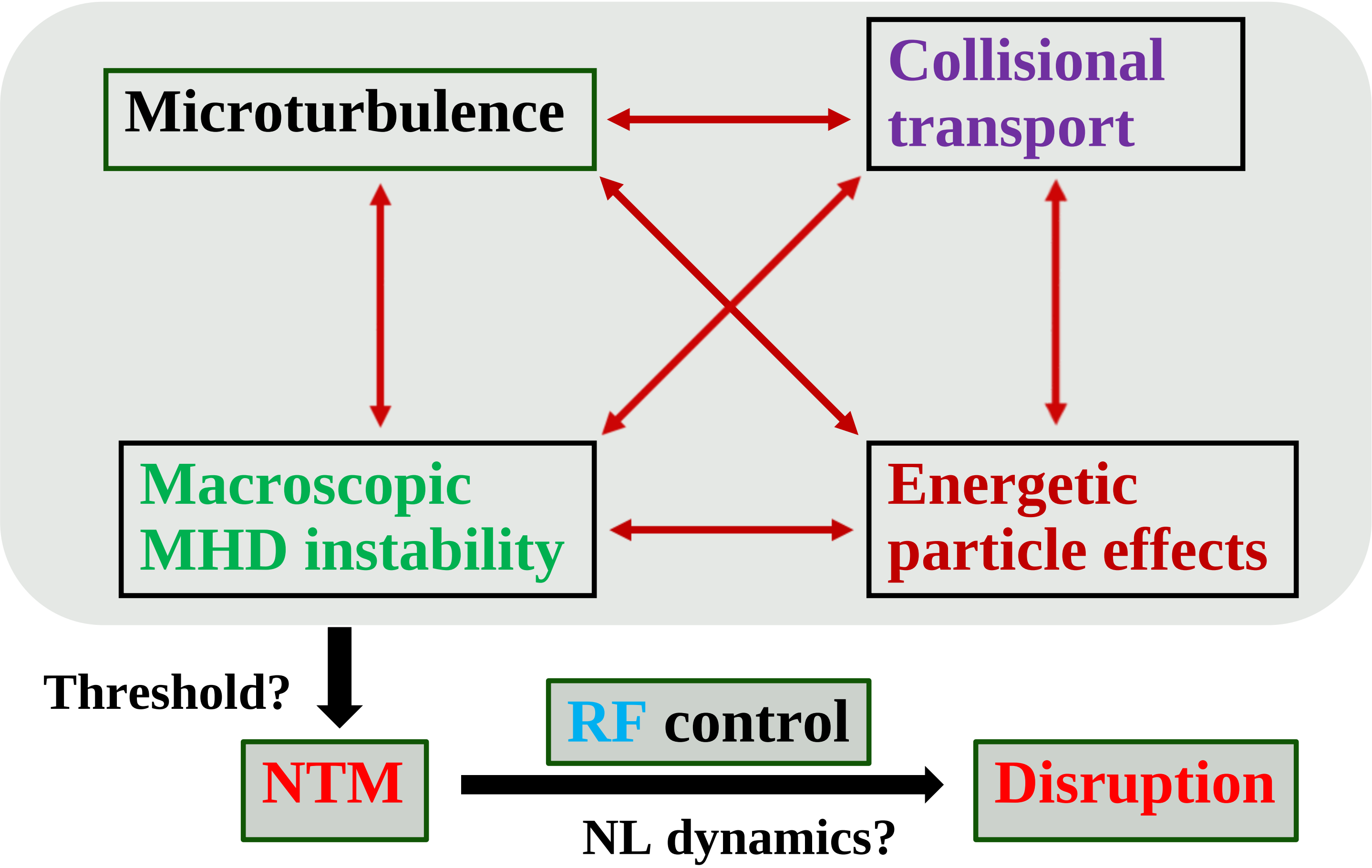
Figure 3: *Multiple physics processes, spatial scales, and temporal scales that must be accounted for in the whole device model of a tokamak [10].*

[Report of the Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences, June 2 – 4, 2015]



[FUSION ENERGY SCIENCES, EXASCALE REQUIREMENTS REVIEW, JANUARY 27–29, 2016]

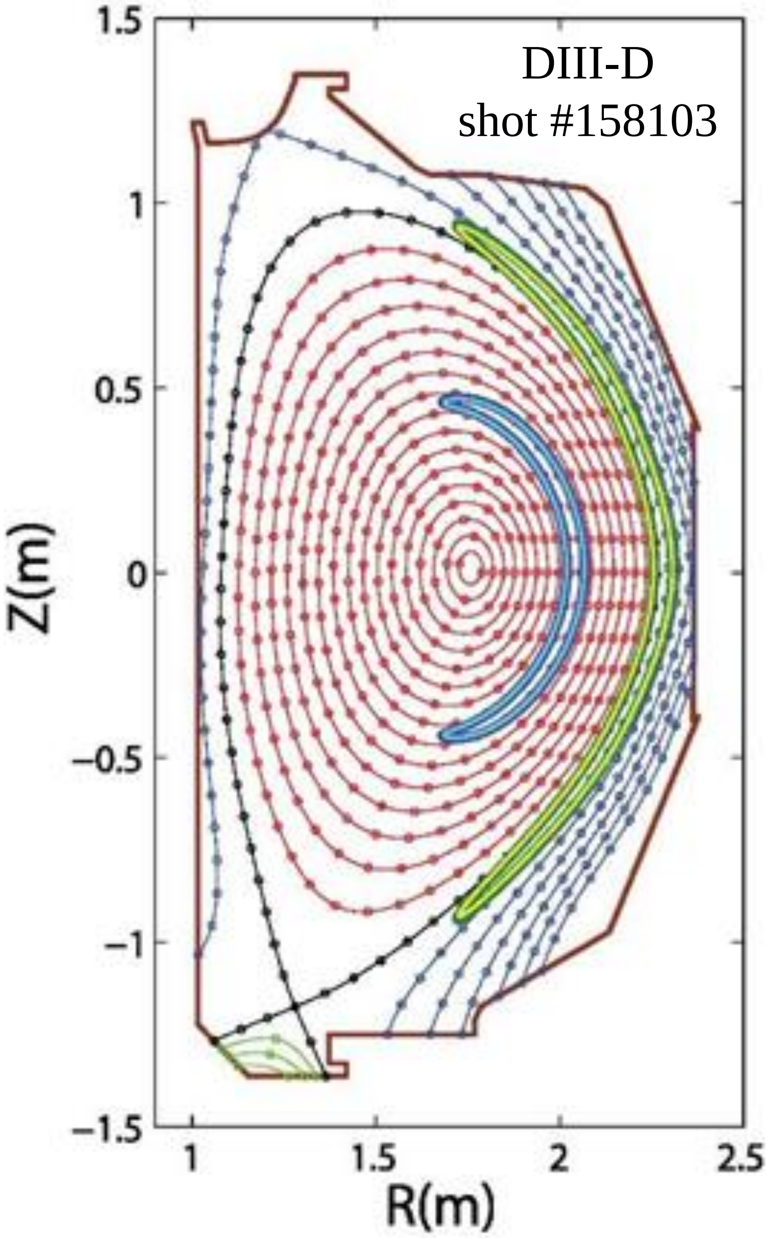
Integrated Simulation Needed to Study Nonlinear Interactions of Multiple Kinetic-MHD Processes



- 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

US Leadership in Fusion Simulation: Most Advanced Tokamak Simulation Capability Developed by DOE Coordinated Collaboration

- Gyrokinetic toroidal code GTC: PPPL 1993-2002, UCI 2002-
- First-principles, integrated simulation capability for nonlinear interactions of multiple kinetic-MHD processes
- Current capability in the central version
  - ✓ Global 3D toroidal geometry & experimental profiles for tokamak, stellarator, FRC
  - ✓ Microturbulence: 5D gyrokinetic ions & electrons, electromagnetic fluctuations, collisionless 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



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

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

Advanced Models for Gyrokinetic Simulation of Kinetic-MHD

- Kinetic effects at microscopic scales and coupling of multiple physical processes play a crucial role in excitation and evolution MHD modes, in fusion, space, and astro plasmas

- Global simulation solving nonlinear gyrokinetic equation, Poisson equation, Ampere's law

$$\frac{\partial F}{\partial t} + (v_\parallel \mathbf{b} + \mathbf{v}_d)\cdot\frac{\partial F}{\partial \mathbf{R}} + \dot{v}_\parallel \frac{\partial F}{\partial v_\parallel} = 0 \qquad \phi - \tilde{\phi} = -\sum_s 4\pi e Z_s \bar{n}_s \qquad \nabla^2 A_\parallel = -\sum_s \frac{4\pi e}{c} Z_s \bar{n}_s u_s$$

- Gyrokinetic system recovers linear MHD modes including Alfven wave, interchange mode, kink mode, kinetic ballooning mode (KBM), resistive & collisionless tearing modes

- Global integrated simulation requires advanced, efficient models

KBM SAW

$$\frac{\omega(\omega-\omega_{*P})}{v_A^2}\nabla_\perp^2\,\delta\phi - i\boldsymbol{B}_0\cdot\nabla\left\{\frac{\boldsymbol{b}_0\cdot\nabla\times[\nabla\times(k_\parallel\,\delta\phi\boldsymbol{b}_0)]}{B_0}\right\}$$

$$-\frac{i\omega}{c}\delta\boldsymbol{B}\cdot\nabla\left(\frac{\boldsymbol{b}_0\cdot\nabla\times\boldsymbol{B}_0}{B_0}\right)$$

kink drive

$$-i\omega\frac{4\pi}{c}\left[\nabla\times\boldsymbol{b}_0\cdot\nabla\left(\frac{\delta P_\parallel}{B_0}\right)+\boldsymbol{b}_0\times\nabla B_0\cdot\nabla\left(\frac{\delta P_\perp}{B_0^2}\right)+\frac{\nabla\times\boldsymbol{b}_0\cdot\nabla B_0}{B_0^2}\delta P_\perp\right]$$

$=0$

interchange drive

*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)*

Outlines

- Integrated fusion simulation requires coordinated program
- Case study: SciDAC ISEP
- International collaborations
- Public-Private partnership

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

SciDAC ISEP: Integrated Simulation of Energetic Particles

- Confinement of energetic particles (EP) is a critical issue for burning plasma experiments 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 when extrapolating from existing fusion devices to ITER
- **EP turbulence and transport**: EP excite meso-scale instabilities (AE) and drive large transport, which can degrade 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 ISEP: new paradigm of nonlinear kinetic simulations of EP turbulence by treating relevant physical processes from micro to macro scales on same footing: non-perturbative, kinetic effects of thermal plasmas

ISEP Objectives Require Coordinated Collaboration

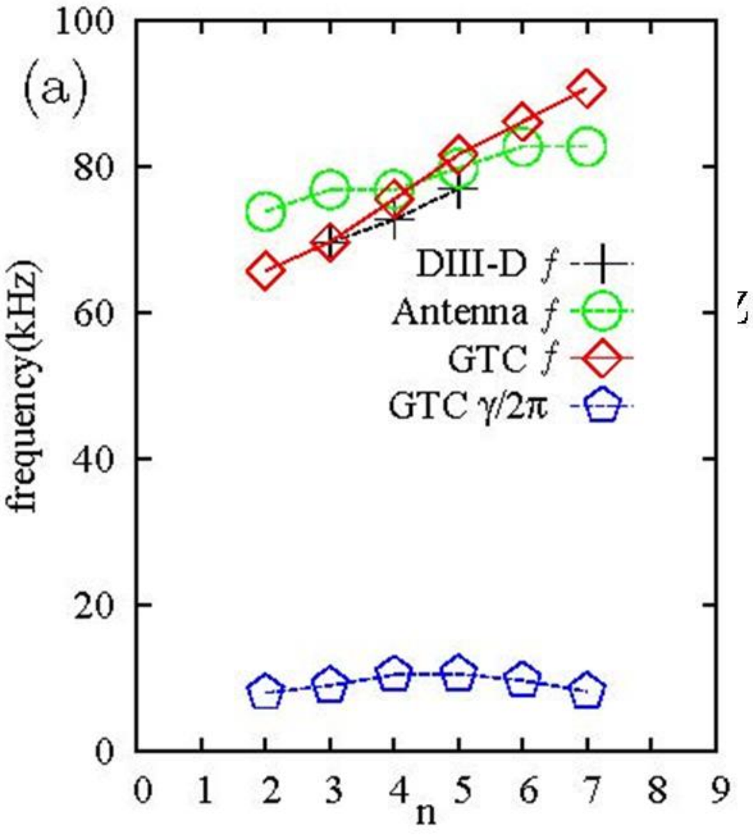
- Study EP physics needed for predictive capability using first-principles simulation
  - EP transport by mesoscale EP turbulence
  - EP coupling with microturbulence and macroscopic MHD modes
- Develop integrated simulation capability for EP physics
  - First-principles ISEP framework based on GTC
- Develop EP module with predictive capability for WDM
  - Reduced EP transport models (CGM, RBQ, machine learning)
  - First-principles ISEP framework
- EP module V&V
- Computational partnership: workflow/data management, solvers, optimization & portability
- Lin, Heidbrink, Chen (UCI), Waltz (GA), Gorelenkov (PPPL), Spong (ORNL), Williams (LBNL), Falgout (LLNL), Tang (PU), Bass (UCSD)

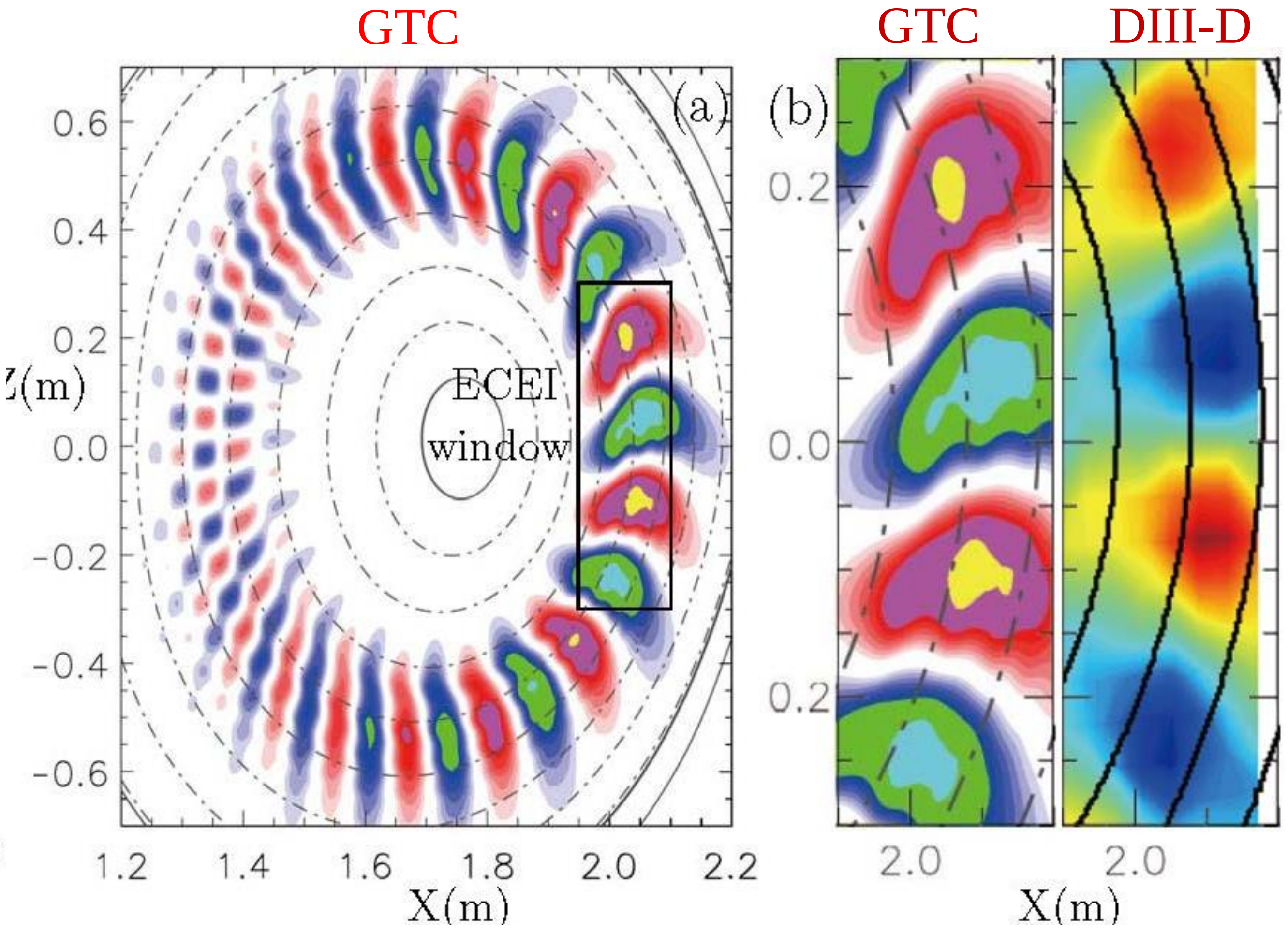
Full Physics Simulation: Comparison of TAE Mode Structures between Simulation & Experiment

- EP non-perturbative effects break radial symmetry of toroidal Alfven eigenmode (TAE), induce TAE radial localization: TAE moves rapidly while thermal plasma profiles barely change
- Thermal ion & electron kinetic effects induce TAE frequency dependence on toroidal mode number n

[Z. X. Wang et al, PRL2013]

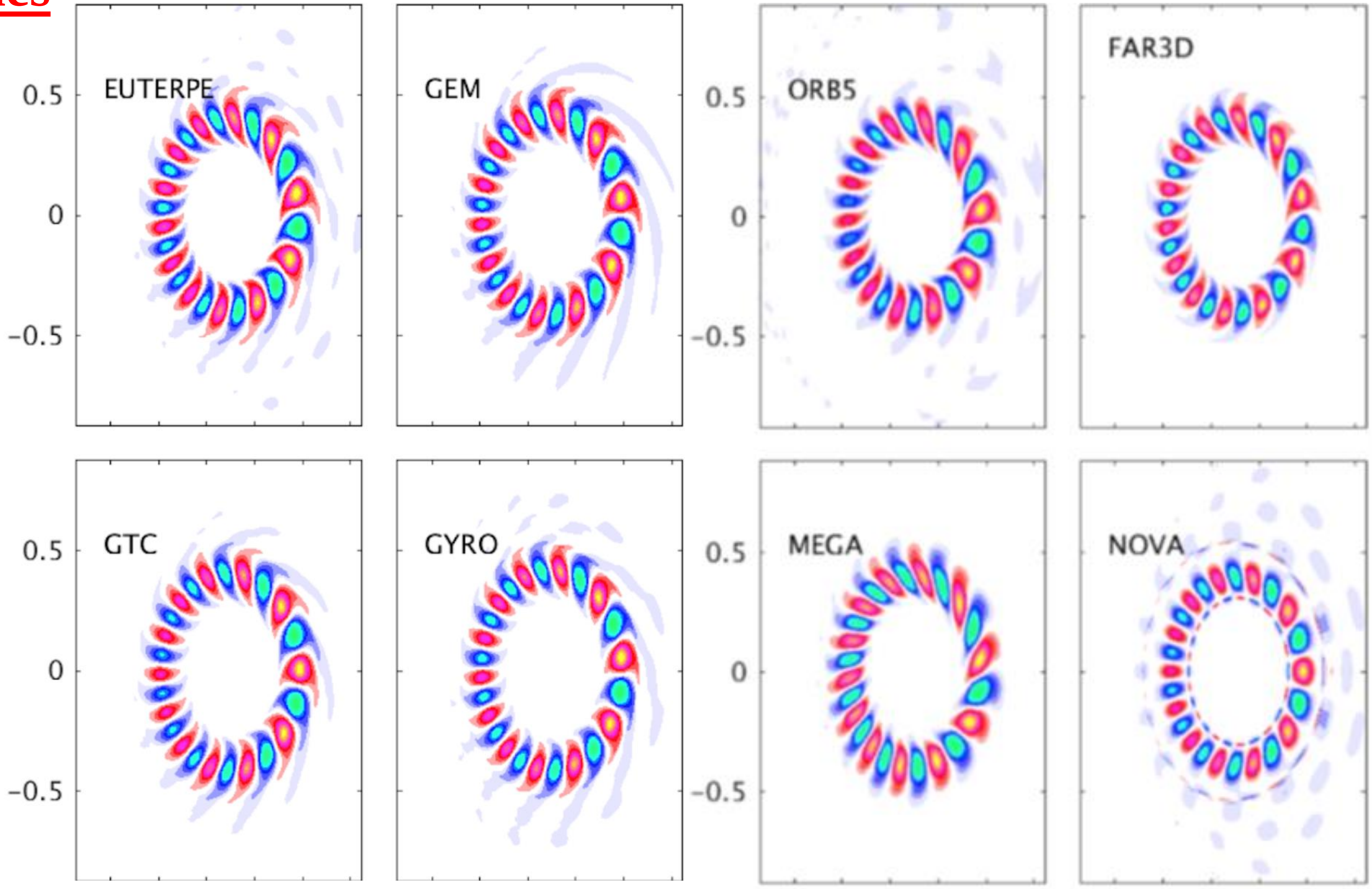
TAE in DIII-D shot # 142111 at 525ms





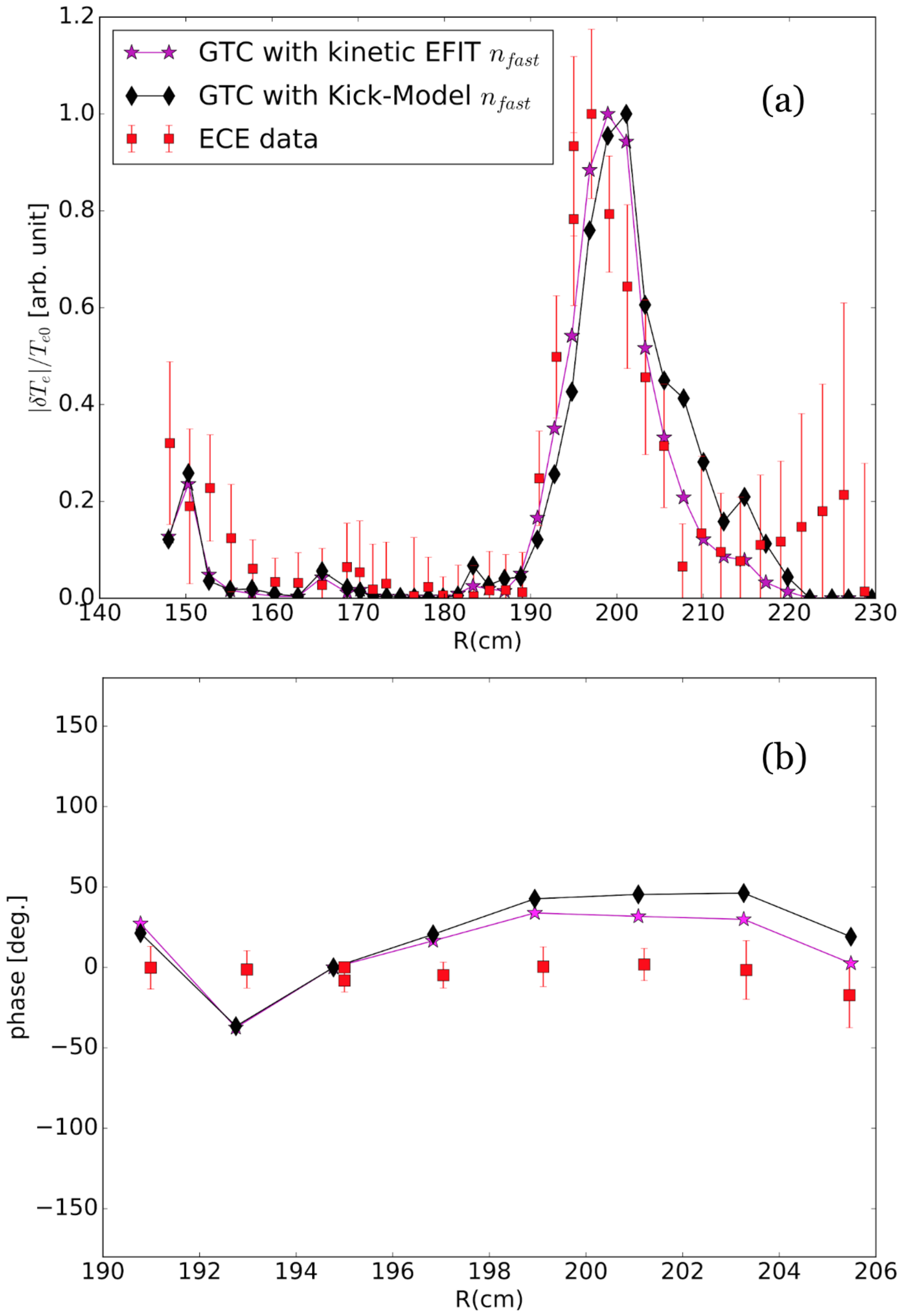
Coordinated Collaboration Facilitates Verification of Gyrokinetic Simulations of Alfven eigenmodes

n=4 reversed shear Alfven eigenmode (RSAE) in DIII-D shot 158243 at 805ms



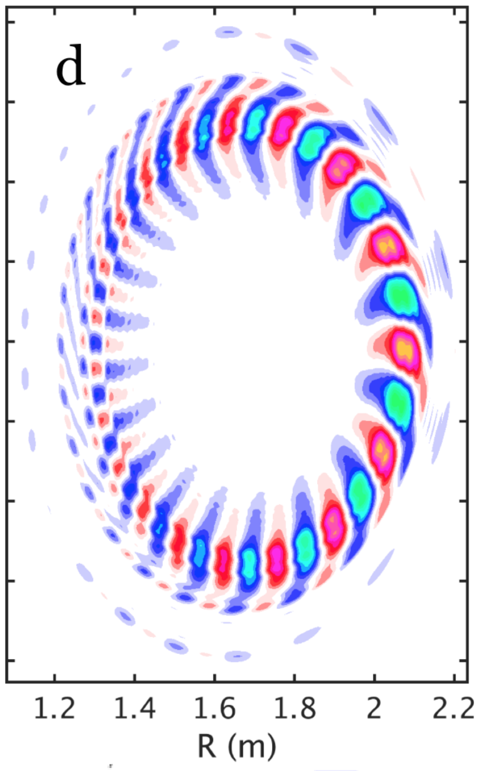
ISEP Validation via Synthetic Diagnostics

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. *[Collins, Heidbrink et al, PRL2016]*

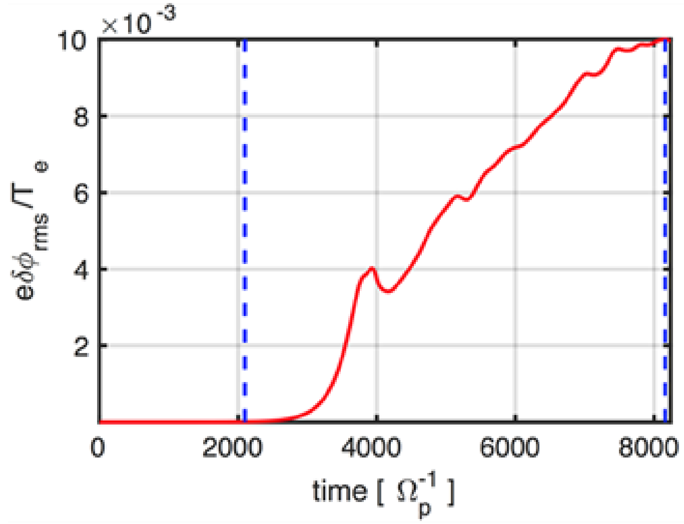


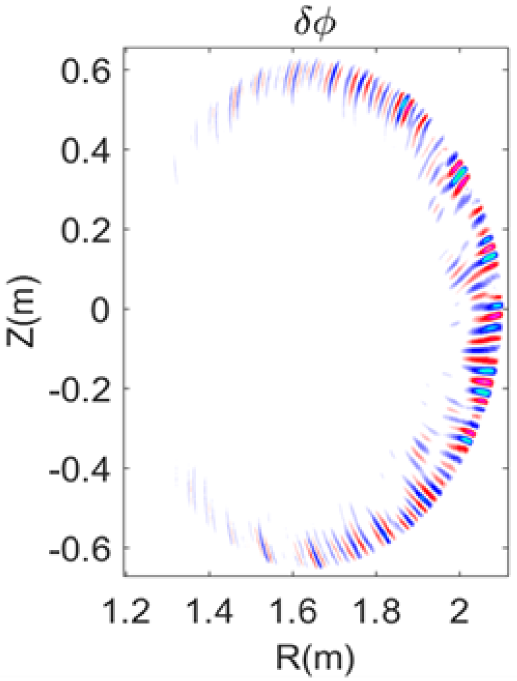
[S. Taimourzadeh et al, NF 2019]

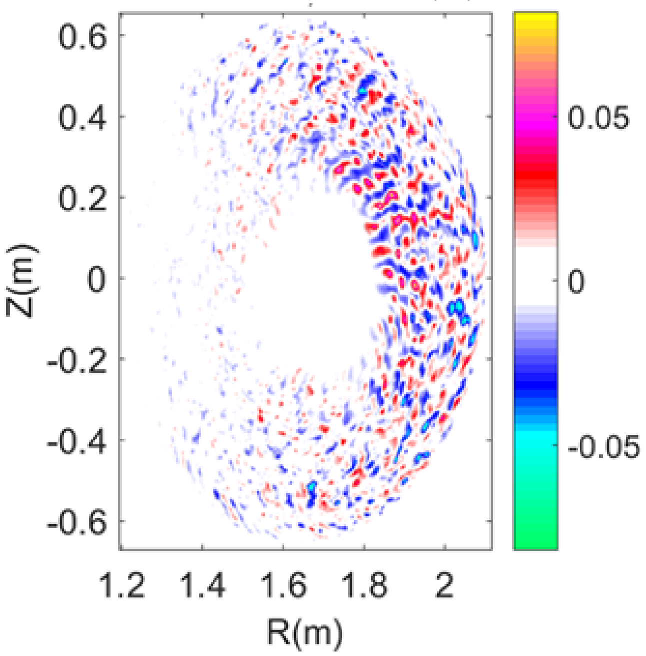
Integrated Simulation of Nonlinear Interaction of RSAE, TAE, Microturbulence



- Using EP profile from kick model, GTC finds strongly unstable RSAE in the core and weakly unstable TAE in the edge of DIII-D shot 158243
- GTC finds strong microinstability in outer edge, nonlinearly spreading to core

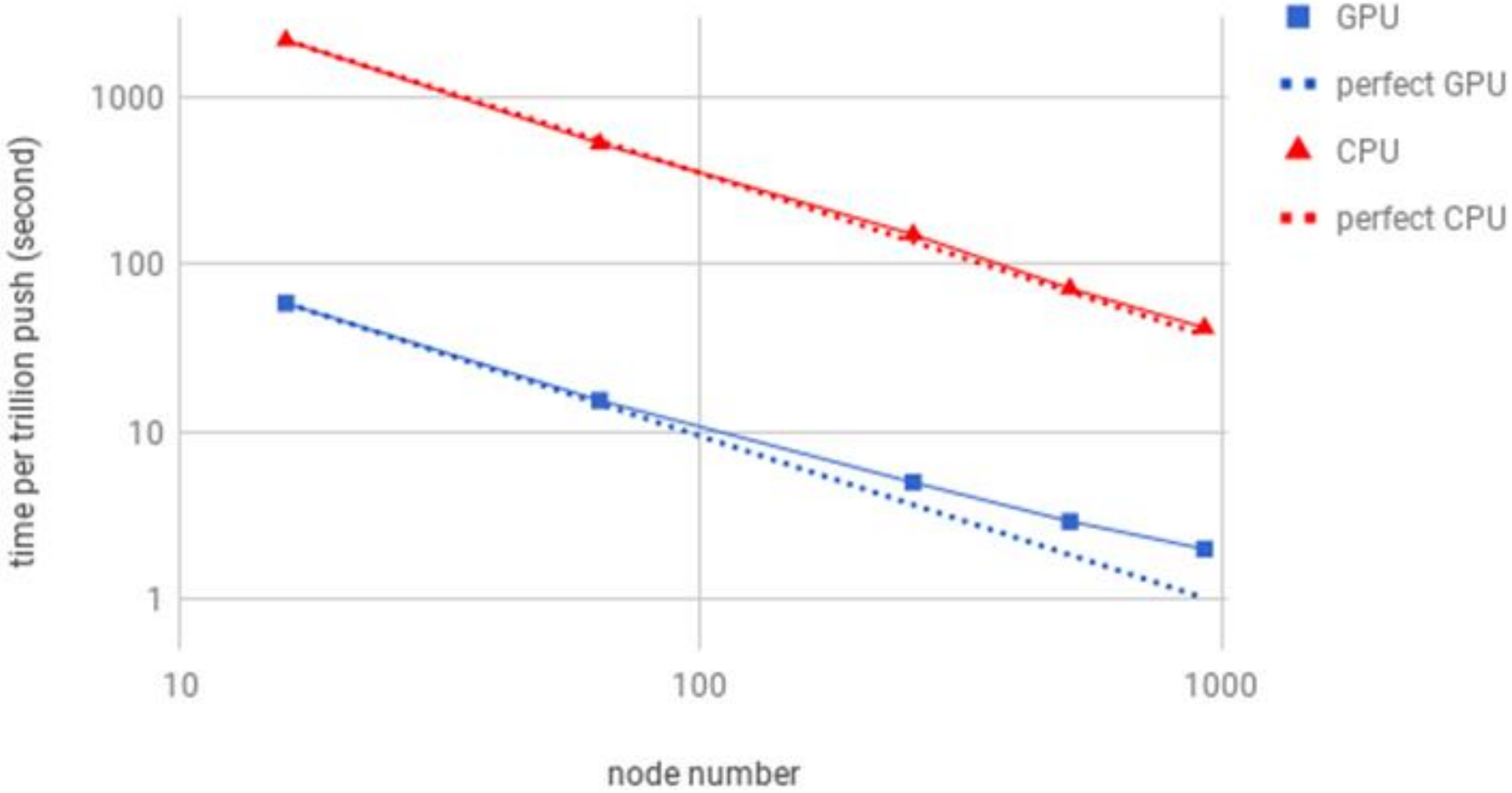






GTC Performance on Pre-exascale Computer Summit

- GTC speeds up 40x from CPU to GPU on 384 GPUs; 20x on 5556 GPUs (>20% of Summit); scalable to 27,456 GPUs (>99% of Summit) in Summit acceptance test
- 3-year INCITE award with ~2% time of Summit ($200M computer)
- Ported to Tianhe-3 prototype



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

HPC Collaborations Enable GTC GPU Optimization

- 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)

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

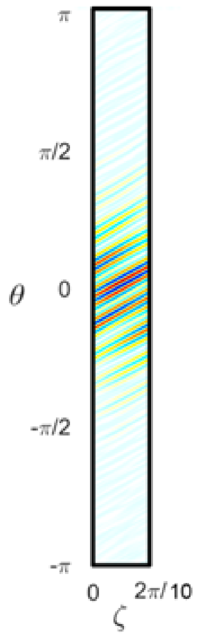
GTC Project Greatly Benefits from Collaborations with ITER-CN Simulation Project

- Collaborations between US SciDAC GSEP/ISEP project (2008-present) and ITER-CN Large Scale Fusion Simulation Project (2013-present)
- GTC team includes ~40 developers and users in US, China, India
- Collaborations resulted in **>50 US-China joint GTC papers** on energetic particle physics, MHD modes, microturbulence, and RF simulations
- **HPC**: GTC porting & optimization on GPU and MIC; used 100s M hours on supercomputers in China: Tianhe-1A, Tianhe-2, ported to Tianhe-3 prototype
- Two GTC HPC talks by international collaborators at supercomputing conferences:

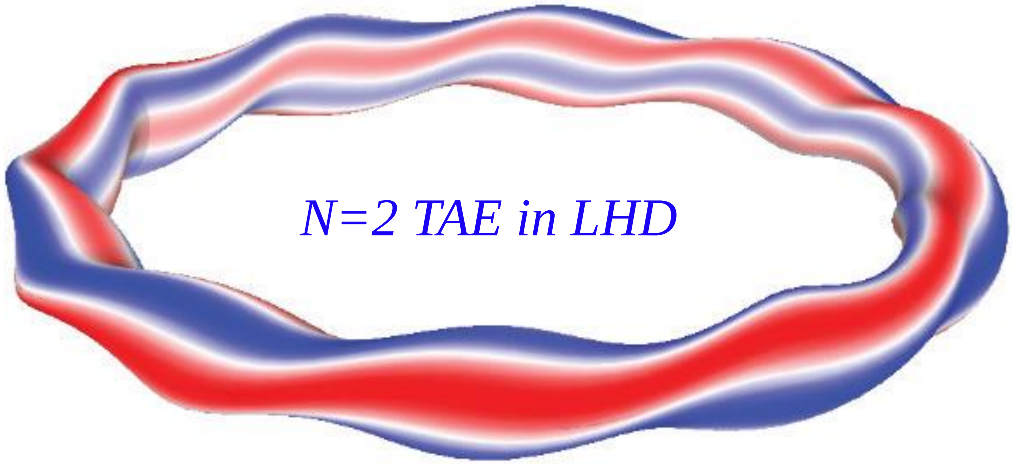
Heterogeneous Programming and Optimization of Gyrokinetic Toroidal Code and Large-scale Performance Test on TH-1A, Xiangfei Meng *et al*, *International Supercomputing Conference*, Leipzig, Germany, 2013

he Gyrokinetic Particle Simulation of Fusion Plasmas on Tianhe-2 Supercomputer, Endong Wang *et al*, Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA), SC2016, Salt Lake City

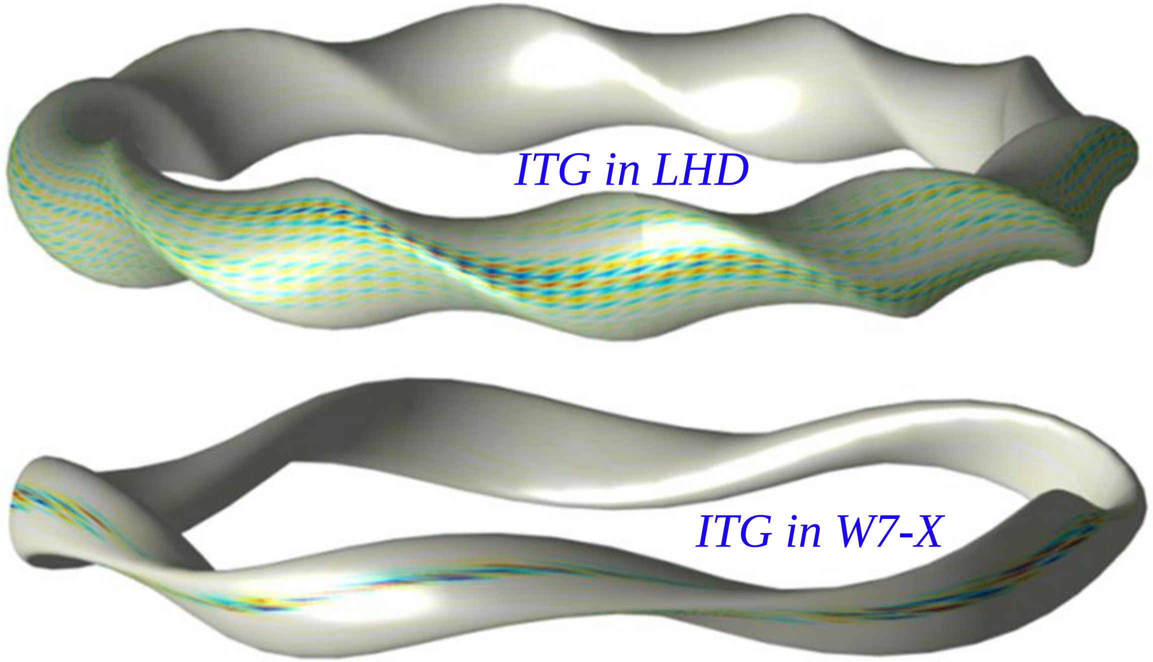
V&V on Unique International Fusion Devices: GTC Simulations of LHD & W7-X Stellarators

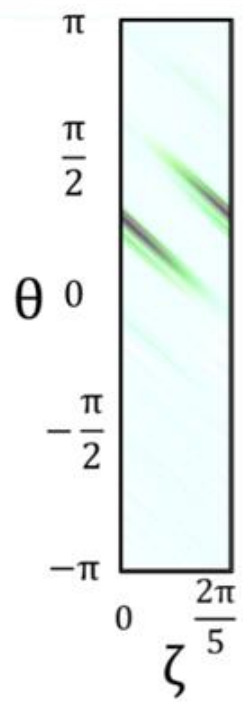


- What are the properties of turbulent transport and energetic particle confinement in stellarators optimized for neoclassical transport?
- GTC linear simulations of toroidal Alfven eigenmode (TAE) in LHD carried out
- GTC growth rate & frequency of ion temperature gradient (ITG) instability agree with 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]

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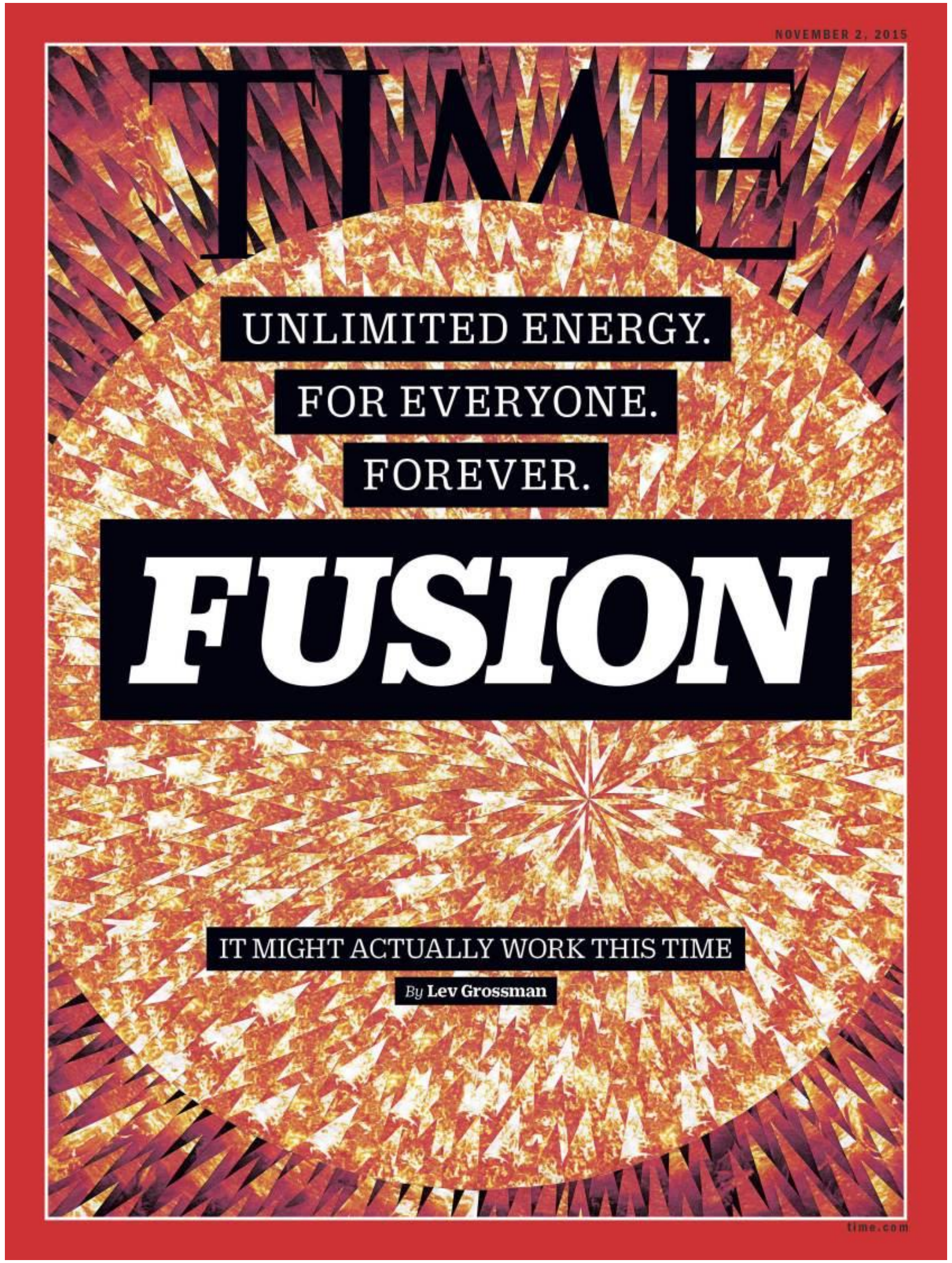
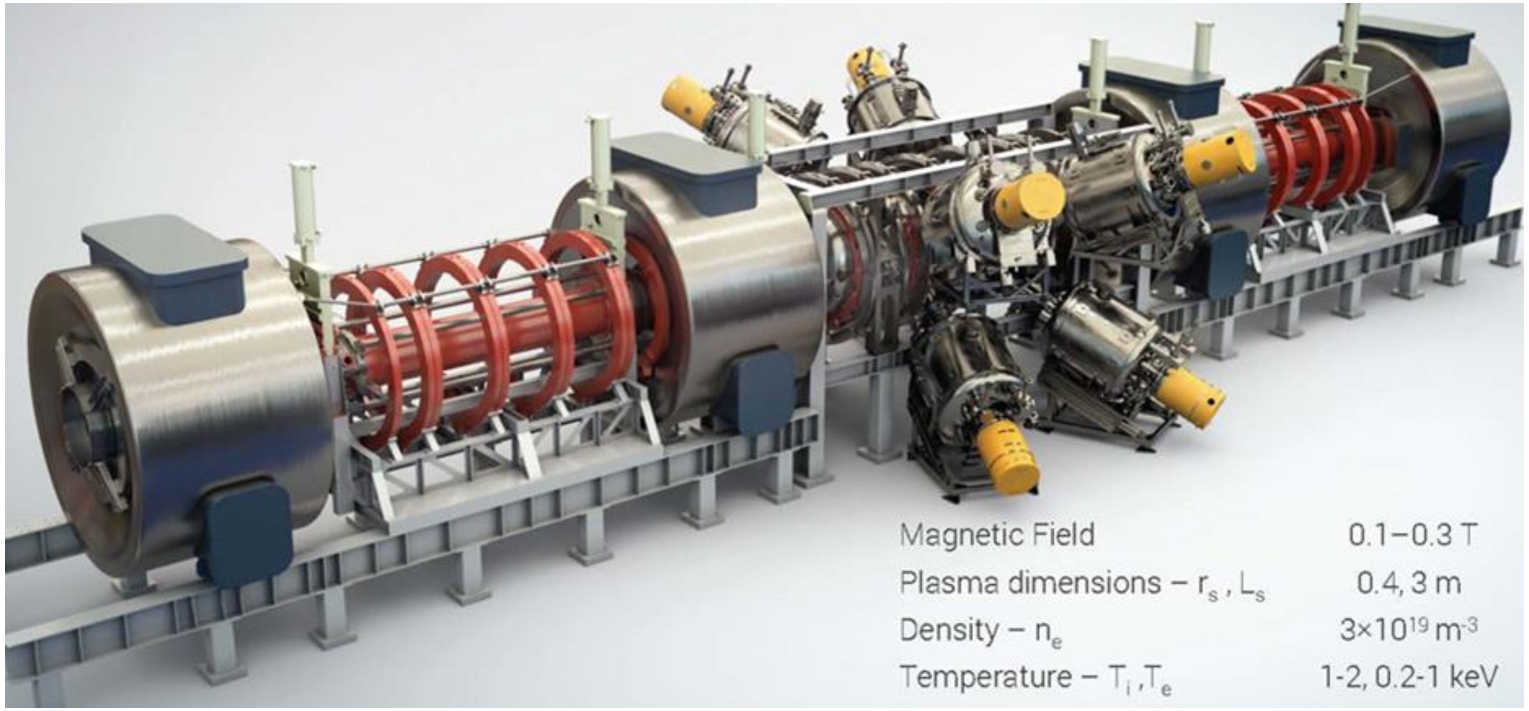
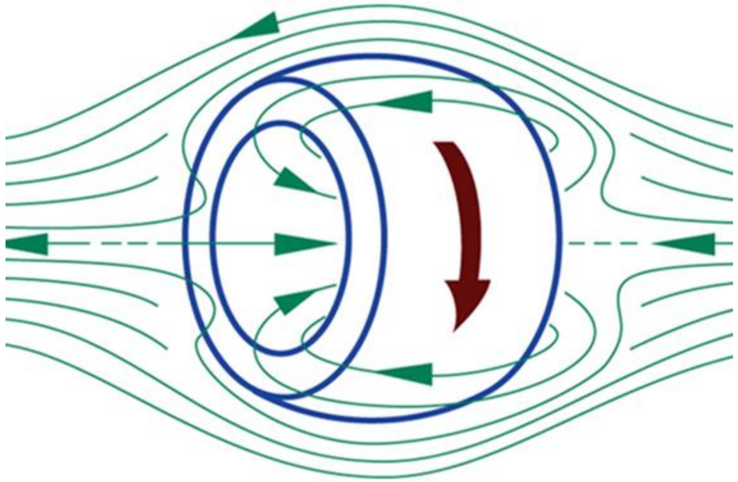
[D. Pace, W. Heidbrink, M. Van Zeeland, 2015]

“IT MIGHT ACTUALLY WORK THIS TIME”







FRC fusion experiment at TAE Technology

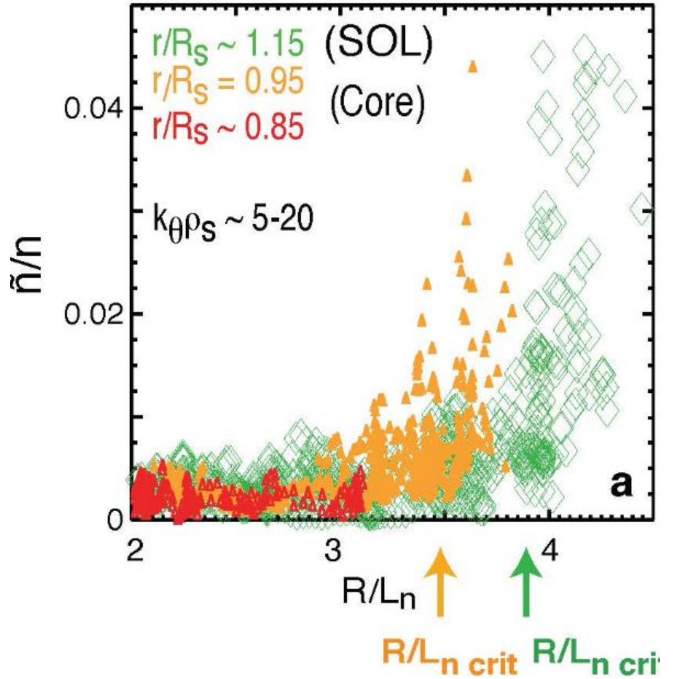
Norman Rostoker
Mchil Binderbauer
Toshiki Tajima

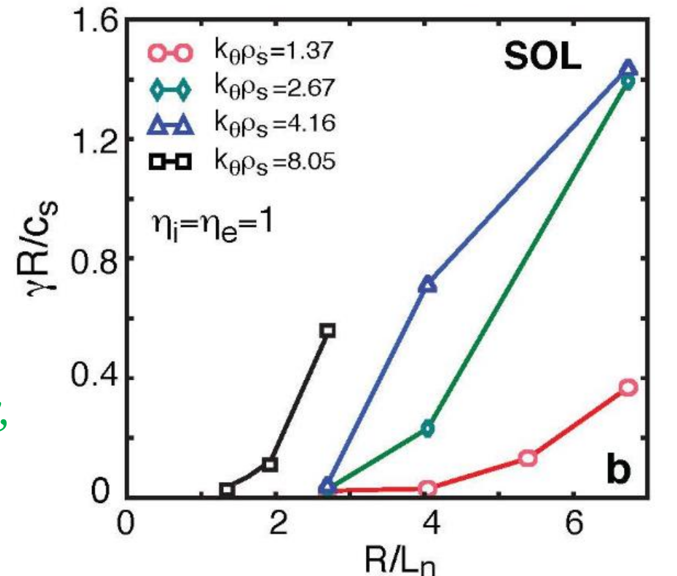
Integrated Simulation of FRC Confinement

- Field-reversed configuration (FRC) emerged as promising alternate concept for compact fusion reactor thanks to remarkable TAE achievements in C-2 series experiments
  - ✓ Reliably controlling macroscopic instability; Surprisingly good ion energy confinement in core
- Can FRC plasmas be heated to and sustained at fusion-relevant regime ($nT\tau$)?
- Thanks to DOE-TAE support, initial progress made in FRC turbulent transport
- However, better understanding of FRC global confinement properties urgently needed
  - ✓ FRC core-SOL coupling? sheared rotation? energetic particle confinement? mirror effects? boundary and divertor physics? electromagnetic fluctuations? high frequency modes? kinetic equilibrium?
- Require multiphysics, multiscale integrated simulation at exascale: IS-FRC
- Leverage tokamak simulation (SciDAC, ECP, CAAR, INCITE, ALCC): physics insights, simulation models, V&V, applied math, computer science
- Can DOE be the steward of IS-FRC, a coordinated public-private partnership?
  - ✓ Building community, coordinated collaborations and goals, computing resources

Simulaitons of FRC Turbulent Transport by DOE-TAE Support

- Effective DOE-TAE joint support for GTC development
  - ✓ Supported by DOE ~100 FTE-year & TAE ~10 FTE-year
- Fruitful UCI-TAE collaborations
  - ✓ Initial physics understanding of FRC turbulent transport
  - ✓ Trained UCI graduate students for TAE research team (Fulton, Lau)
  - ✓ Initial development of TAE turbulence simulation code ANC
- Physics: microscopic driftwave expected to be unstable 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





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)*

Workforce in fusion simulation in high demand:
UCI theses during past 5 years

- Fusion simulation faces challenges in workforce development: competing talent in job market, unconventional career path for interdisciplinary researchers, shrinking/aging plasma faculty
- Sam Taimourzadeh (2018): *Gyrokinetic simulation of RMP effects on turbulent Transport in DIII-D tokamak edge;* Employer, Toyota *Inc*.
- Calvin Lau (2017, Rostoker Fellowship): *Gyrokinetic simulation of driftwave instability in FRC;* Employer, TAE Technologies *Inc*.
- Onnie Luk (2016, Gates Millennium Scholars), *Gyrokinetic simulation of nonlinear interaction of kinetic shear Alfven waves;* Employer, Max-Planck Institute for Plasma Physics, Garching, Germany.
- Joseph McClenaghan (2015), *Gyrokinetic simulation of current-driven instabilities;* Postdoc, General Atomics.
- Daniel Fulton (2015, Rostoker Fellowship), *Gyrokinetic simulation of driftwave instability in FRC;* Employer, TAE Technologies *Inc*.
- Zhixuan Wang (2014), *Gyrokinetic simulation of TAE in DIII-D;* Postdoc, General Atomics.

Conclusions

- Coordinated collaborations, SciDAC program (2001-present), are crucial for the success of ISEP project
  - Build a critical mass for sustainable and collaborative code development to provide a first-principles EP module of WDM for burning plasmas
  - Facilitate model development, V&V, physics discovery, and building user community
  - Enhance fusion-HPC collaboration for new technologies (e.g., ML), evolving hardware & software ecosystem
- ISEP benefits greatly from international collaborations: HPC, V&V etc
- Public-private partnership: growing area for fusion simulation
- Fusion simulation needs workforce development