An overview of recent results from the SCREAM SciDAC project

D.P. Brennan
Plasma Physics Laboratory
Princeton University

Presented as a Research Review Seminar
Princeton Plasma Physics Laboratory
June 15, 2018

SCREAM is addressing all the primary issues identified in REs

- Critical questions on runaway electron physics are driving the research
  - Scattering of runaways by whistler waves, kinetic instabilities (could increase cyclotron losses and facilitate mitigation)
  - Magnetic surface break up and and reformation.
  - Impurity penetration to core of plasma
  - The poloidal flux change required for an e-fold in the number of energetic electrons when $E_{||} >> E_{ch}$.
  - The spatial and temporal localization of relativistic electron losses.
  - What can be learned about runaways during the non-nuclear phase of ITER operations.
  - Mitigation methods (injection of particles, injection of cyclotron waves, induced currents in walls)

- Here we focus on a few selected highlights in some of these areas
  - A comprehensive overview would be prohibitively long

Great overview of RE issues:
A. H. Boozer, "Pivotal issues on relativistic electrons in ITER," Nuclear Fusion 58, 036006 (2018).

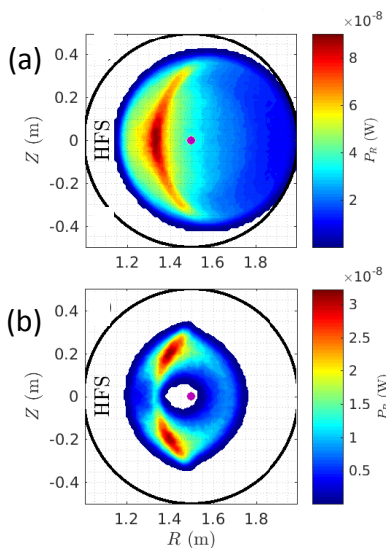
Outline: SCREAM highlights in theory and simulation of REs

- Runaway electron generation
  - Full orbit simulations of runaway electrons with KORC
  - The backward Monte Carlo and Adjoint methods for runaway probability
  - The lifetime of runaways
  - Runaway vortex
- Thermal quenches and magnetic surface breakup
  - Reduced modeling of VDEs
  - Disruptions and RE Modeling with NIMROD and RE Orbit Modeling
- Mitigation via impurity injection
  - In MHD simulations of MGI and SPI with RE tracers
  - Theoretical efforts to better understand experiments
- Whistler wave scattering of runaway electrons
  - Explaining experimental observations of spontatneous onset
  - Exploring the use of wave launching to mitigate REs
- Advanced Vlasov-Fokker-Planck solvers
  - Conservative relativistic Fokker-Planck solvers
  - Conservative adaptive algorithms for the Landau collision integral
  - Conservative Hamiltonian Vlasov integrators
- Highlights of future directions

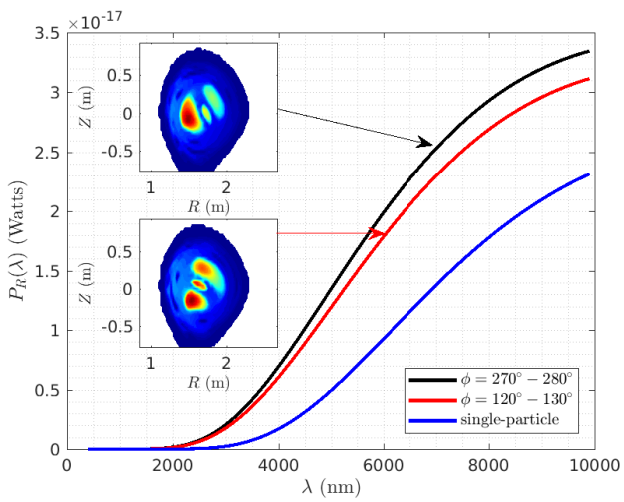
Numerical simulation of runaway electrons: 3-D effects on synchrotron radiation (SR)

Significance and Impact

- Understanding SR is important because radiation damping is one of the main energy loss mechanisms of runaway electrons and also because SR is routinely used as an experimental diagnostic.
- Our study showed the key role played by trapped-particles dynamics and 3-D magnetic field effects including magnetic islands and stochasticity.
- Applications to DIII-D quiescent plasmas used to validate and point out potential limitation of current models of pitch angle dynamics.



Distinct radiation patterns of: (a) passing and (b) trapped runaway electrons exhibiting two "hot" spots at the tips of the banana orbits.



Impact of 3-D magnetic islands structures and stochasticity on SR. Inserts show the spatial distribution of SR at different toroidal angles. Neglecting orbit effects (blue lines) significantly underestimates SR.

Scientific Achievement

- Used KORC, an ORNL recently developed 6-D kinetic particle-based code, to perform a first of a kind study of 3-D magnetic field geometry and orbit effects on synchrotron radiation (SR)
- Quantified radiation emission of trapped particles
- Studied role of magnetic islands and stochasticity on the 3-D spatial distribution of SR and power spectra
- Modeled SR on DIII-D quiescent plasmas.

Research Details

- SR of trapped particles exhibits nontrivial spatial distributions and has a strong dependence on orbit effects.
- Computed RE orbits in stochastic magnetic fields characteristic of disrupted plasmas during thermal quench phase.
- Magnetic fields computed using the MHD code NIMROD
- Very good agreement with DIII-D quiescent plasmas experiments.
- First of a kind runaway model validation study

D. del-Castillo-Negrete, L. Carbajal, D.Spong, and V. Izzo. Invited presentation APS-DPP 2017. Physics of Plasmas 25, 056104 (2018).

The Backward Monte Carlo (BMC) Method for Runaway Electron Simulations on HPC

Guannan Zhang (ORNL) and Diego del-Castillo-Negrete (ORNL)

ASCR and FES joint effort at ORNL for SCREAM

Objectives / Novel Ideas

- Our goal is to significantly improve the accuracy and efficiency of Monte Carlo simulation of runaway electron (RE) dynamics for disruption mitigation in fusion tokamaks.
- Our main idea is to develop a novel mathematical theory and algorithm, i.e. the backward Monte Carlo method, to compute dynamical probability of runways electron.
- We will integrate the BMC method into the ORNL-developed particle code KORC, for the purpose of simulating full-orbit RE probabilities on OLCF supercomputers.

Impact

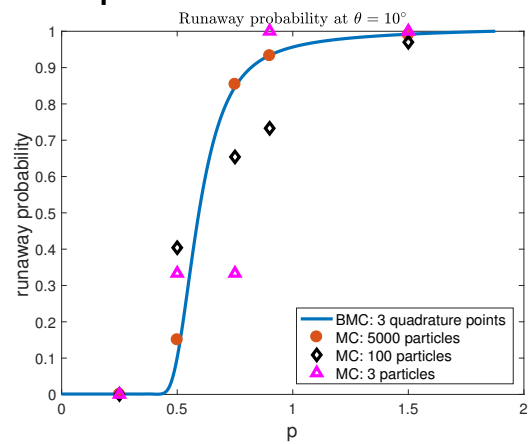
- **Efficiency:** the BMC method can achieve the same accuracy with significantly reduced computational cost, e.g., *reducing from 5000 particles (for MC) to 3 particles (for BMC)*.
- **Scalability:** the BMC algorithm share *the same scalability* as the standard Monte Carlo methods on HPCs.
- **Flexibility:** the BMC algorithm can be easily coupled with any particle code for runaway electron simulation.
- **Applicability**: the BMC method can help physicists efficiently predict the performance of new disruption mitigation strategies

Publication

G. Zhang and D. del-Castillo-Negrete, *A backward Monte-Carlo method for time-dependent runaway electron simulations*, **Physics of Plasmas**, 24, 092511 (2017).

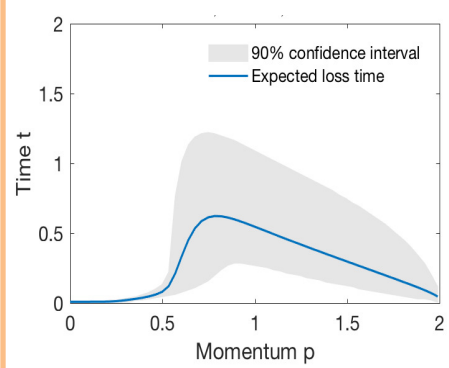
Accomplishments

Comparison between MC and BMC



- **Accuracy**: the BMC method with 3 particles achieves the same accuracy as the standard MC method with 5000 particles;
- **Efficiency**: the MC method with a similar cost to the BMC method (i.e., with 3 or 100 particles) leads to totally incorrect answers.

Uncertainty analysis of RE dynamics



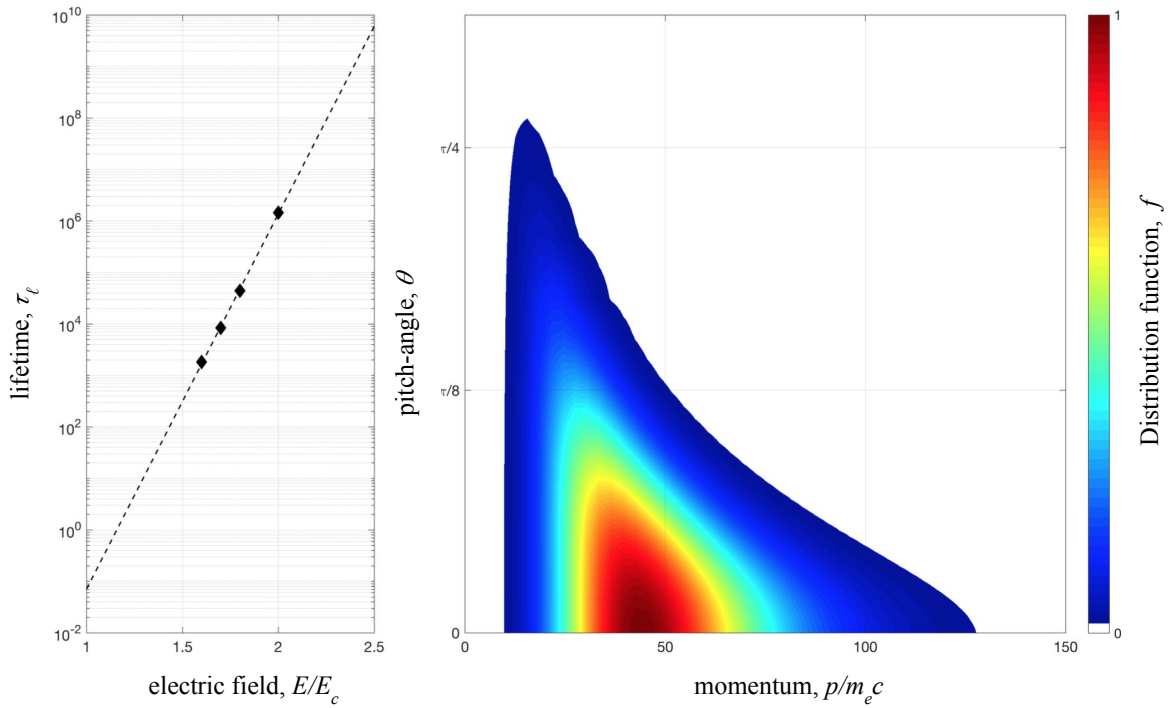
We did uncertainty analysis of RE dynamics by computing statistics using the BMC method, including:

- Expected runaway time
- Expected loss time (left figure)
- Confidence interval of the loss time (left figure)

U.S. DEPARTMENT OF ENERGY | Office of Science

Lifetime and Universal Distribution of Seed Runaway Electrons

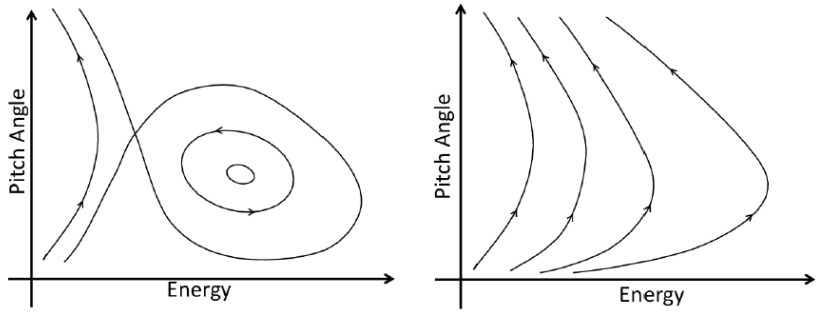
A.K. Fontanilla, B.N. Breizman, Phys. Plasmas 24, 112509 (2017).
Featured in AIP Scilight, Nov. 2017



The lifetime (left) of runaway electrons increases exponentially with the inductive field which facilitates the onset of avalanche. The runaway seed forms a quasi-stationary distribution (right) in momentum-space due to the balance between the inductive drive, collisional friction, and synchrotron drag.

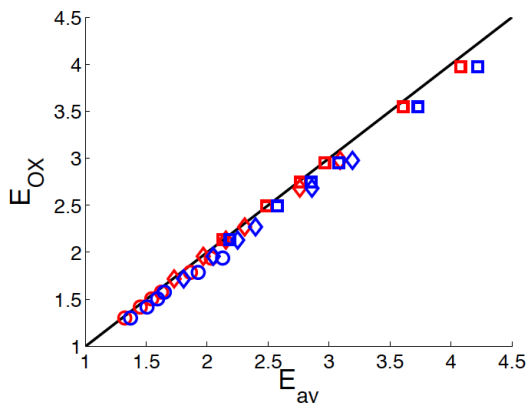
Avalanche Threshold: simple predictive model based on runaway momentum space topology

Large E → Primary runaway vortex → Avalanche

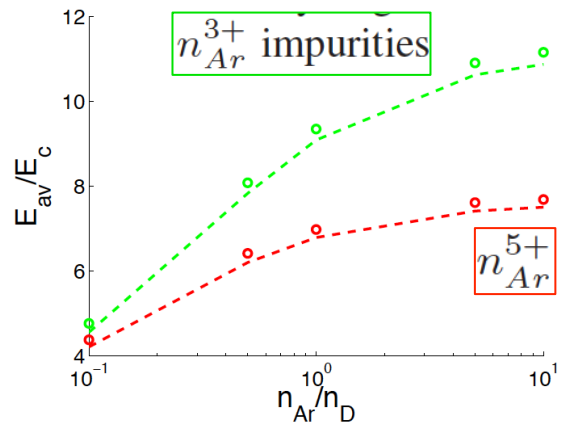


Small E → No primary runaway vortex → No avalanche

McDevitt, Guo, Tang, "Relation of the Runaway Avalanche Threshold to Momentum Space Topology" Plasma Physics and Controlled Fusion 60 (2), 024004 (2018).



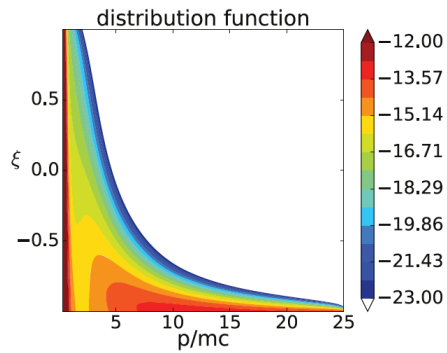
Z=1-10 and α=0.025-0.3

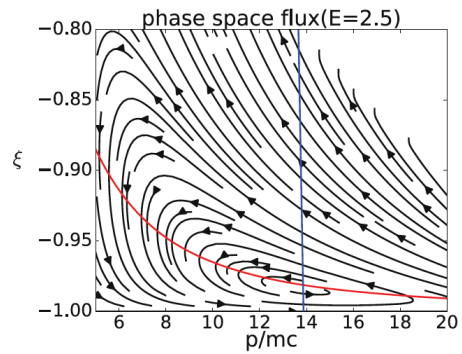


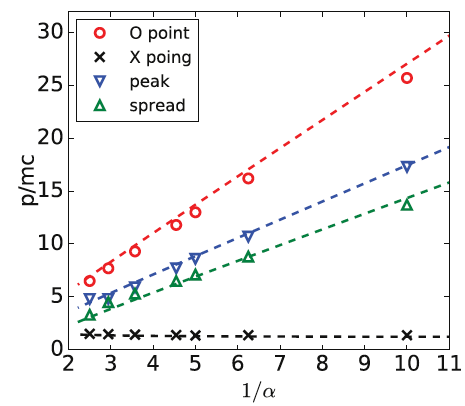
Including partial screening + inelastic collisions with high-Z impurity

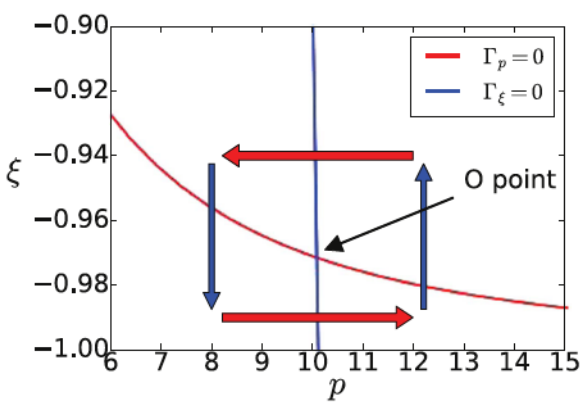
Runaway energy and pitch distribution saturation

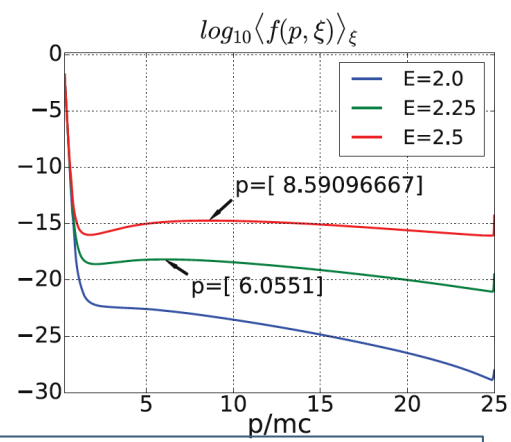
- Due to radiation damping, runaways can saturate in energy and pitch ➔ Runaway vortex → sets the primary runaway mean energy, the energy spread, and the bump in energy for pitch-integrated distribution.

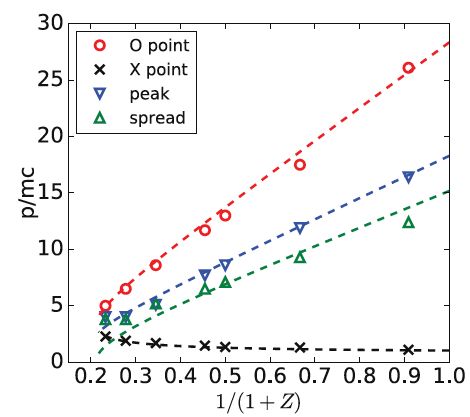












Guo, McDevitt,Tang, "*Phase-space dynamics of runaway electrons in magnetic fields*," PPCF 59, 044003 (2017)

$\alpha \equiv \tau_C / \tau_S =$ collisions/synchrotron

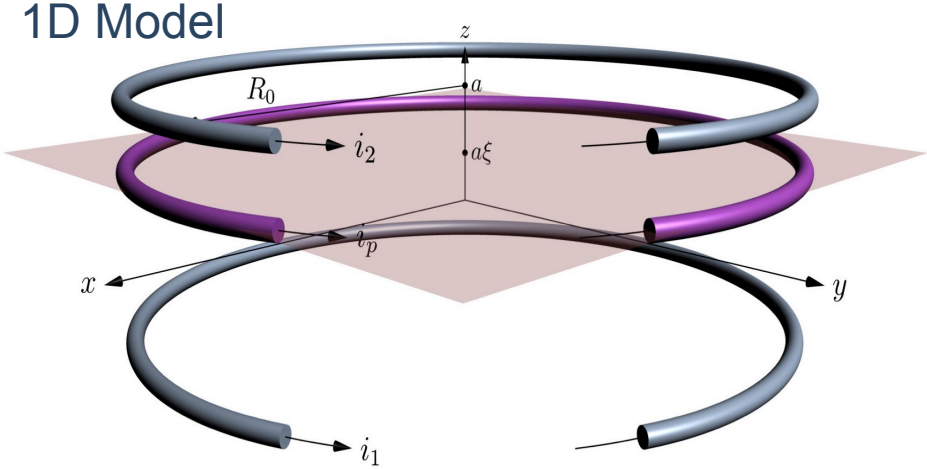
Outline: SCREAM highlights in theory and simulation of REs

- Runaway electron generation
  - Full orbit simulations of runaway electrons with KORC
  - The backward Monte Carlo and Adjoint methods for runaway probability
  - The lifetime of runaways
  - Runaway vortex
- Thermal quenches and magnetic surface breakup
  - Reduced modeling of VDEs
  - Disruptions and RE Modeling with NIMROD and RE Orbit Modeling
- Mitigation via impurity injection
  - In MHD simulations of MGI and SPI with RE tracers
  - Theoretical efforts to better understand experiments
- Whistler wave scattering of runaway electrons
  - Explaining experimental observations of spontatneous onset
  - Exploring the use of wave launching to mitigate REs
- Advanced Vlasov-Fokker-Planck solvers
  - Conservative relativistic Fokker-Planck solvers
  - Conservative adaptive algorithms for the Landau collision integral
  - Conservative Hamiltonian Vlasov integrators
- Highlights of future directions

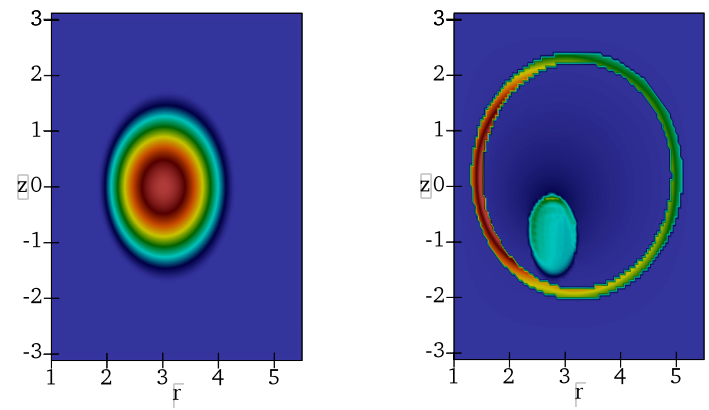
Model of Vertical Plasma Motion During The Current Quench

D.I. Kiramov and B.N. Breizman, Phys. Plasmas 24, 100702 (2017)

1D Model



2D Model

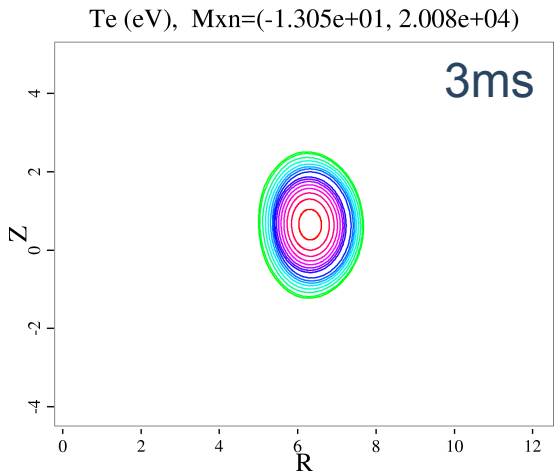


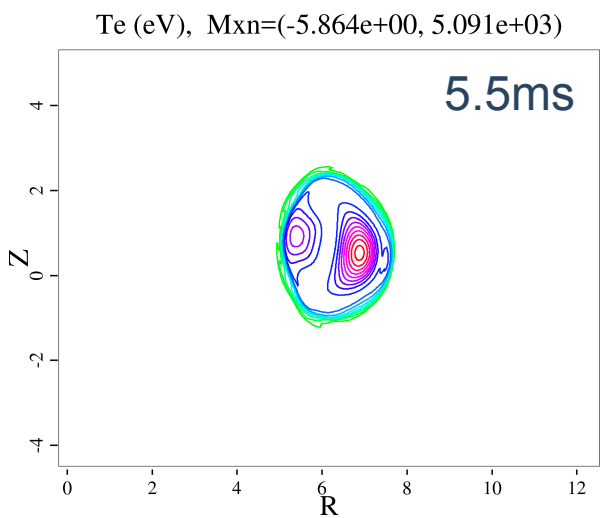
- The plasma current decay time is shorter than the wall resistive time in cold VDEs.
- Cold VDEs are characterized by a monotonic relation between the plasma current and plasma vertical displacement.

2D cold VDE code is being developed to

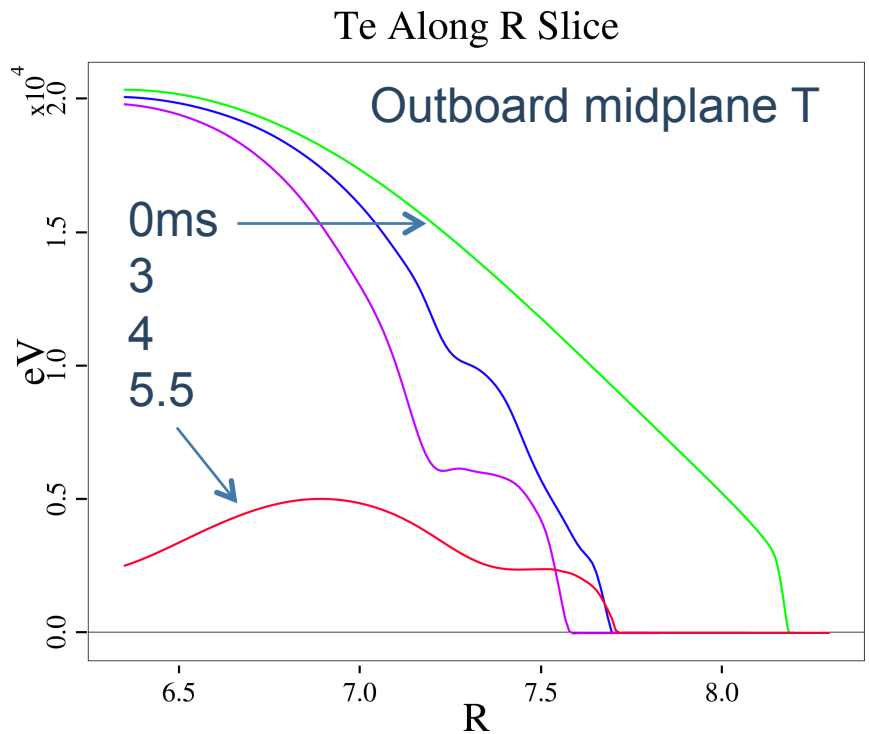
- Highlight key physics of 2D force-free plasma motion
- Amend numerical codes accordingly

Disruptions and RE Modeling with NIMROD: Simulations of SPI and runaway confinement in ITER thermal quench





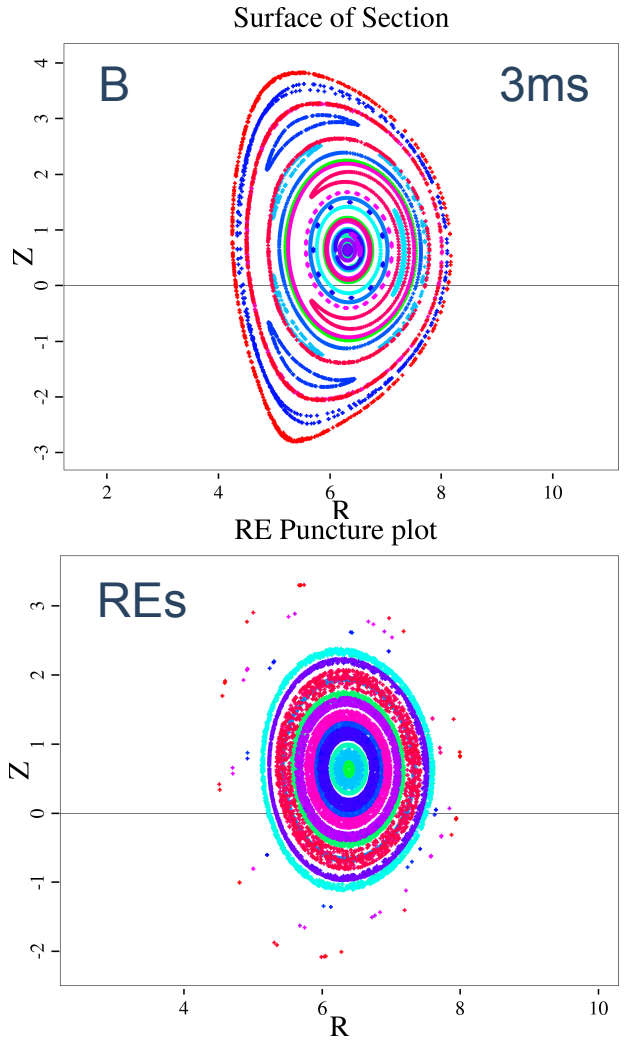
Initially 15MA Q=10 ITER Equilibrum
0.5kPam^3 pure Ne pellet shatters into 125 fragments
Outboard midplane, spread out along single 1.5m beam



60% T quench, all fragments ablate by 4.5ms

C.C. Kim, in preparation 2018.

REs are found to be insensitive to islands and somewhat robust to stochasticity



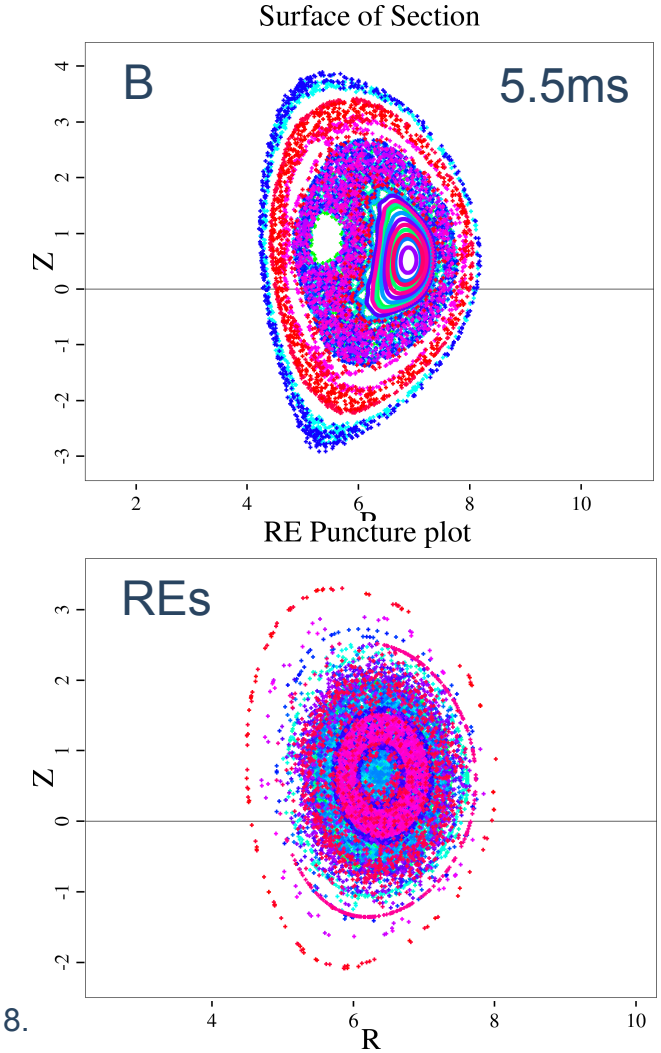
RE tracers accelerated in full fields for 30μs. Similar to work of V. Izzo.

Caveat: pitch scatter in $v_{||}$ but not in mu

Find some quasi confined orbits in stochastic region.

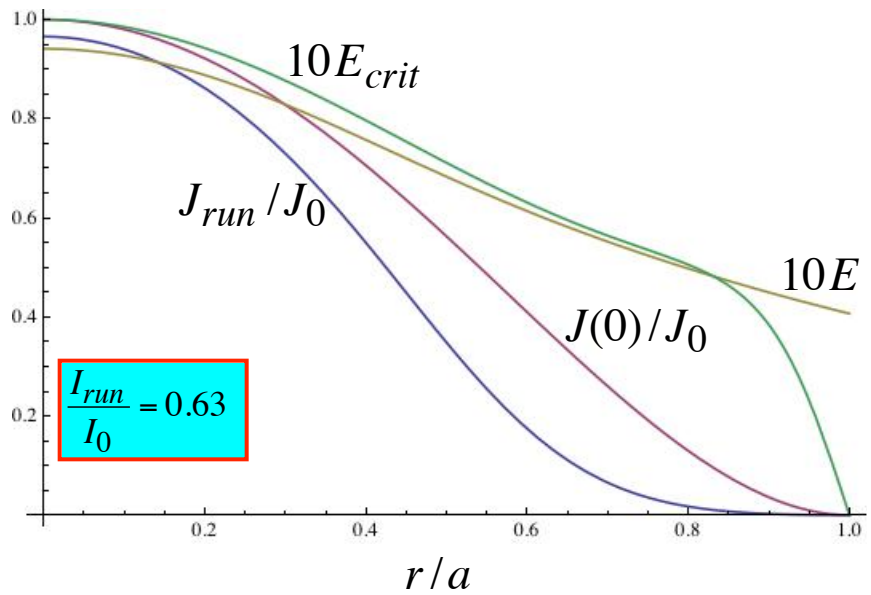
Note: Poincare points are at fixed ϕ crossing
RE trace plots are at fixed time intervals

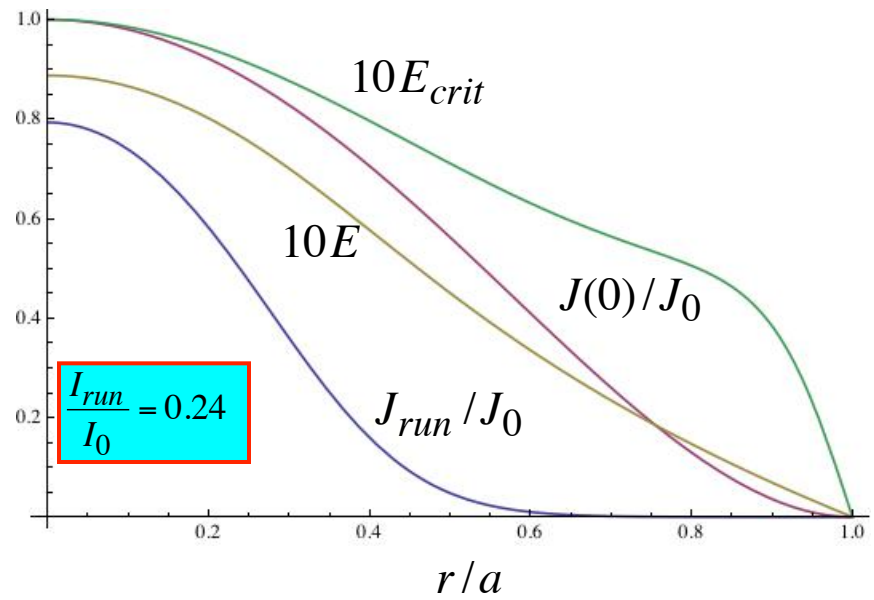
C.C. Kim, in preparation 2018.



With No Gas Injection in ITER Plateau-Phase Runaways Decay Slowly even for Two Extremely Different Types of Boundary Conditions

- **Current density and electric field profiles in ITER 100 ms after Runaways form I_0 = 11 MA, I_{seed} = 1.1 kA, and central E_{crit} = 0.1 V/m (n_{e14} = 1)**





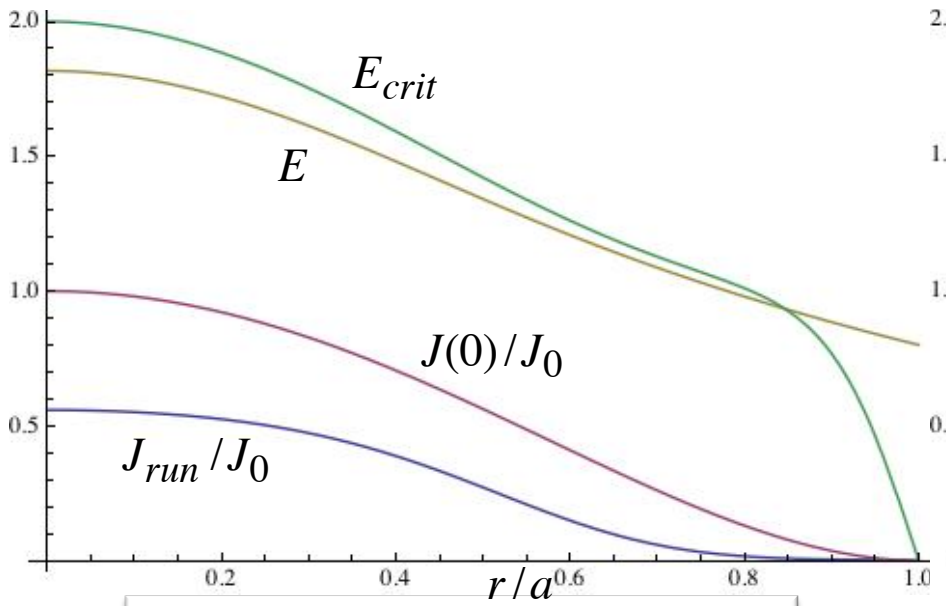
Passive OH-Coils and wall time = 0

Ideal wall on plasma surface, E = 0 at surface

→ **Forcing E = 0 at surface causes less RE current conversion than a resistive wall because plasma current is partly transferred to wall. But E is still close to E_{crit} keeping decay rate slow in the core, but at edge current has already dissipated.**

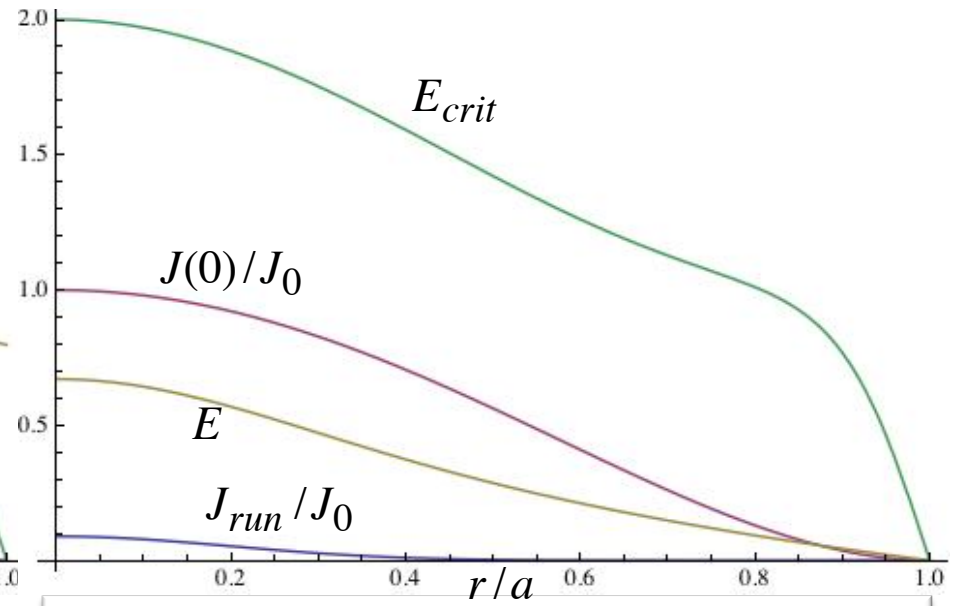
But Surface Boundary conditions Have a Great Effect on Dissipation rate of Plateau-Phase Runaways with a modest amount of Late Gas Injection

- **Current density and electric field profiles 300 ms after Runaways form**
  I_0 = 11 MA, I_{seed} = 1.1 kA, and central E_{crit} = 2 V/m (n_{e14} = 20 for D_2)



Passive OH-Coils and wall time = 0

$$\frac{I_{run}}{I_0} = 44.6\%$$



Ideal wall on plasma surface, E = 0 at surface

$$\frac{I_{run}}{I_0} = 1.98\%$$

→ **Forcing E = 0 at surface causes faster RE current decay because interior driving E-field is forced to be well below E_{crit}.**

Outline: SCREAM highlights in theory and simulation of REs

- Runaway electron generation
  - Full orbit simulations of runaway electrons with KORC
  - The backward Monte Carlo and Adjoint methods for runaway probability
  - The lifetime of runaways
  - Runaway vortex
- Thermal quenches and magnetic surface breakup
  - Reduced modeling of VDEs
  - Disruptions and RE Modeling with NIMROD and RE Orbit Modeling
- Mitigation via impurity injection
  - In MHD simulations of MGI and SPI with RE tracers
  - Theoretical efforts to better understand experiments
- Whistler wave scattering of runaway electrons
  - Explaining experimental observations of spontatneous onset
  - Exploring the use of wave launching to mitigate REs
- Advanced Vlasov-Fokker-Planck solvers
  - Conservative relativistic Fokker-Planck solvers
  - Conservative adaptive algorithms for the Landau collision integral
  - Conservative Hamiltonian Vlasov integrators
- Highlights of future directions

Now clear that whistler scattering is critical physics needed to interpret runaway electron experiments

D. Spong, PRL 2018

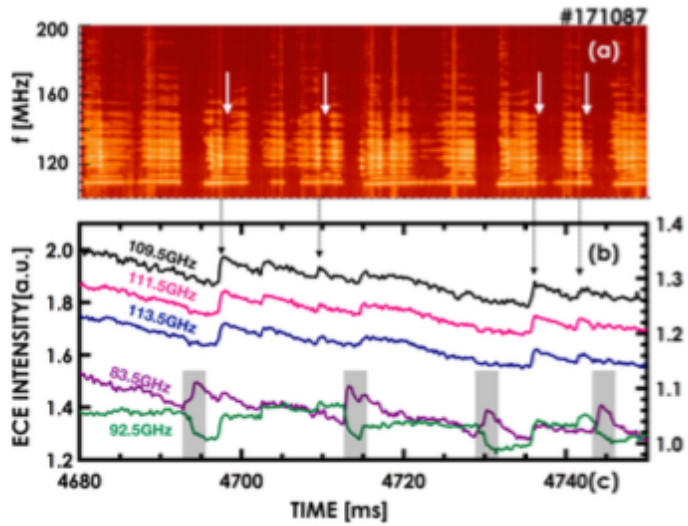


Figure 6 – Time evolution of (a) 100 to 200 MHz magnetic fluctuation power spectra; (b) ECE intensity at 83.5, 92.5, 109.5, 111.5, and 113.5 GHz. Dashed arrows in (b) are times at which the ECE and whistler amplitudes peak; Solid arrows in (a) are times at which whistler amplitudes drop. The grey shaded bars are intervals of n = 1 sawtooth activity.

C.Liu PRL 2018

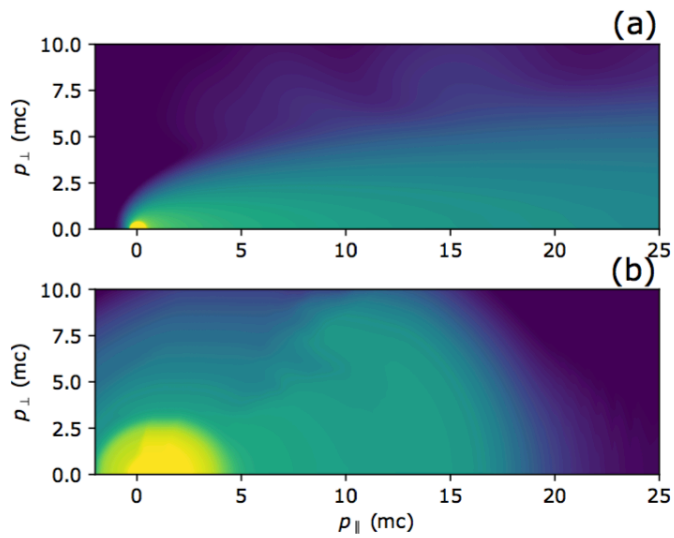


Figure 1: Scattering of runaway electron distribution function by whistler waves (b), compared to simulation without kinetic instabilities (a).

Both the whistler wave amplitudes and the ECE signals show cyclic behavior, and have strong correlations with each other. Modeling and simulation indicates whistler scattering key.

D. Spong, Post-Deadline Invited Talk, APS-DPP 2017

D.A. Spong "First direct observation of runaway electron-driven whistler waves in tokamaks", accepted for publication Phys. Rev. Lett.

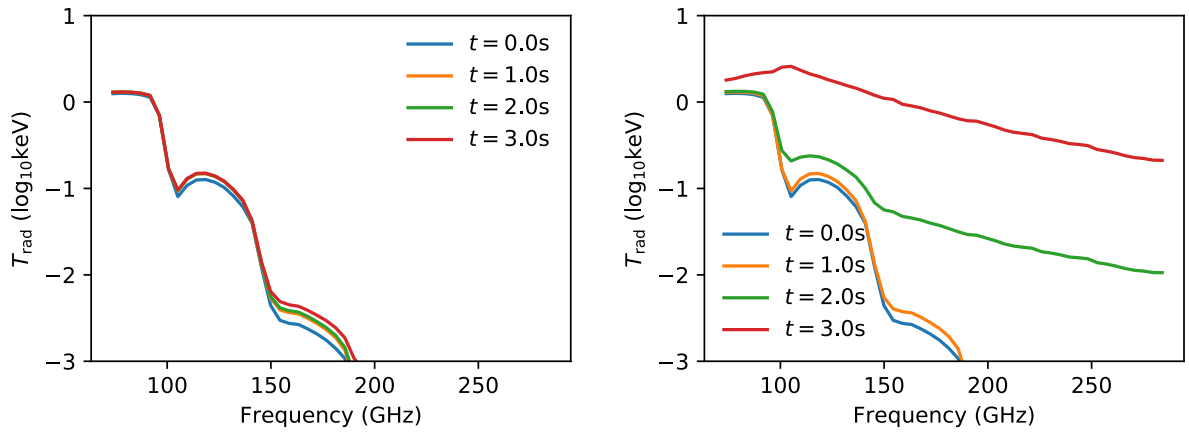
Including modeling contributions from SCREAM

Quasilinear whistler interaction with REs reproduces prompt growth and broad spectrum in ECE

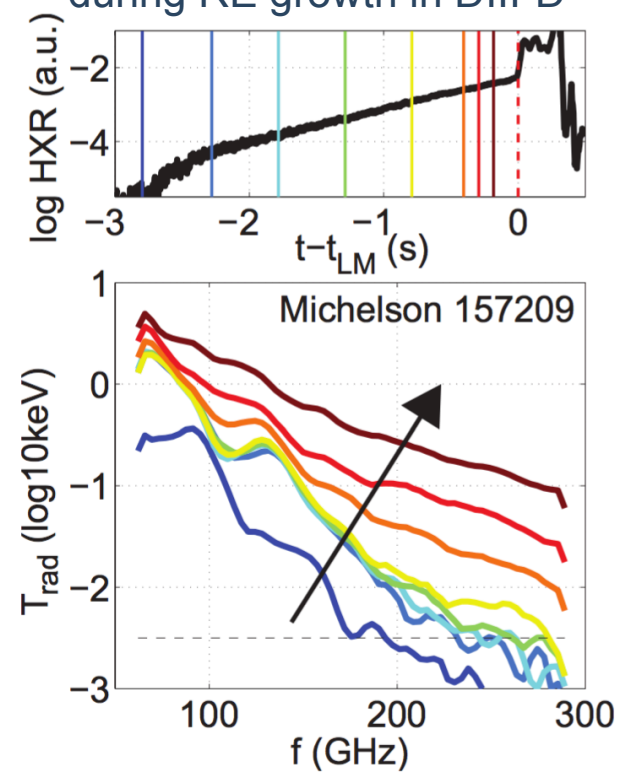
Key result: whistler scattering is largely responsible for the dynamic growth of energy spectrum observed in QRE experiments

In addition: cyclical behavior and fast growth of higher harmonics predicted

Simulated ECE spectrum



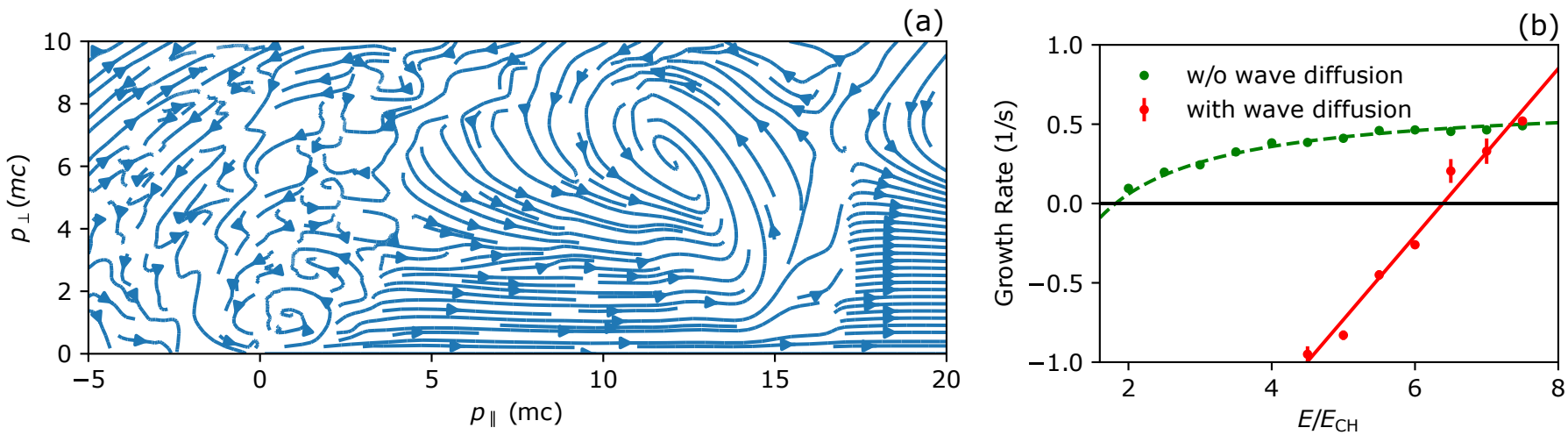
ECE Spectrum evolution during RE growth in DIII-D



Chang Liu, Lei Shi, Eero Hirvijoki, Dylan P. Brennan, Amitava Bhattacharjee, Carlos Paz-Soldan, Max E. Austin, "The effects of kinetic instabilities on the electron cyclotron emission from runaway electrons," accepted for publication Nucl. Fusion, arXiv:1803.09897 (2018).

Quasilinear whistler interaction and phase space vortices explain critical E field puzzle

C. Liu et al, “Role of kinetic instability in runaway electron avalanche and elevated critical electric fields” arXiv:1801.01827, accepted for publication PRL 2018



Experimental measurements of critical electric field for runaway have consistently been found to be 2x-3x higher than theory predicts with radiation and avalanche effects alone.

Explained by quasilinear whistler wave interaction – could be critical effect for ITER.

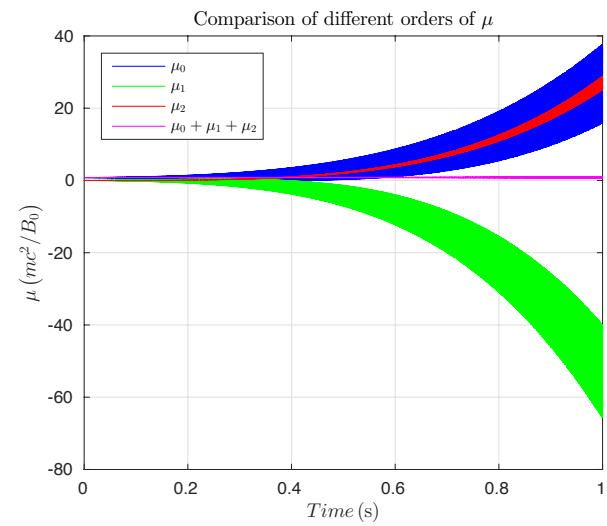
Invariance of magnetic moment explains collisionless pitch-angle scattering

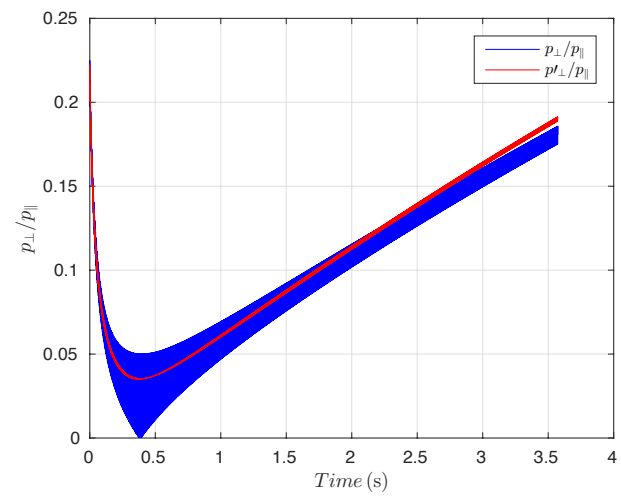
Full-orbit simulations[1,2] reveal break-down of the standard magnetic moment μ_0 and collisionless pitch-angle scattering.

The standard μ_0 is only the lowest-order term in the asymptotic series for the full magnetic moment. Higher order guiding center analysis suggests the full magnetic moment is still conserved to large extent.

Using the conservation of μ with second order corrections, the spreading of pitch angle found in simulations can be explained.

By going into higher order and considering $p_{//} \gg p_{\perp}$ for runaway electrons, we obtain a new set of guiding-center coordinates for runaway electrons, which can be the basis of a GC simulation framework[3].





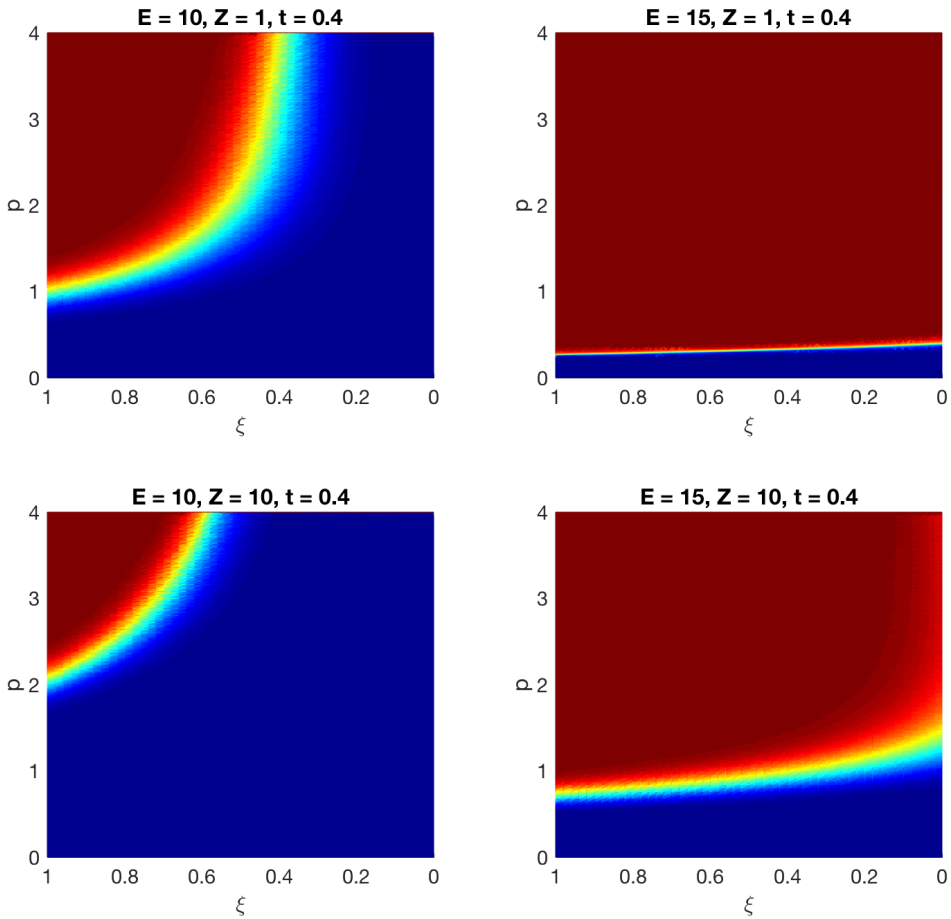
[1]J. Liu, Y. Wang, and H. Qin, Nucl. Fusion 56, 064002 (2016).
[2]L. Carbajal, D. del-Castillo-Negrete, D. Spong, S. Seal, and L. Baylor, Phys. Plasmas 24, 042512 (2017).
[3]C. Liu, H. Qin, E. Hirvijoki, Y. Wang, and J. Liu, ArXiv:1804.01971 (2018).

A fluid-kinetic framework for self-consistent runaway-electron simulations

Target: MHD disruption simulations with self-consistent, kinetic treatment of runaway electrons

Method[1,2]: one-fluid equations and kinetic equation for runaway electrons coupled in terms of transition probabilities between the kinetic tail and bulk fluid

Key aspect: time-dependent transition probabilities computed deterministically from the stochastic trajectories of particles[3].



[1]E. Hirvijoki, C. Liu, Q. Zhang, D. del-Castillo-Negrete, and D. Brennan, ArXiv:1802.02174 (2018).
[2]E. Hirvijoki, Phys. Plasmas 25, 040702 (2018), ArXiv:1801.03084.
[3]Q. Zhang and D. del-Castillo-Negrete, Phys. Plasmas 24, 092511 (2017), ArXiv:1708.00947.

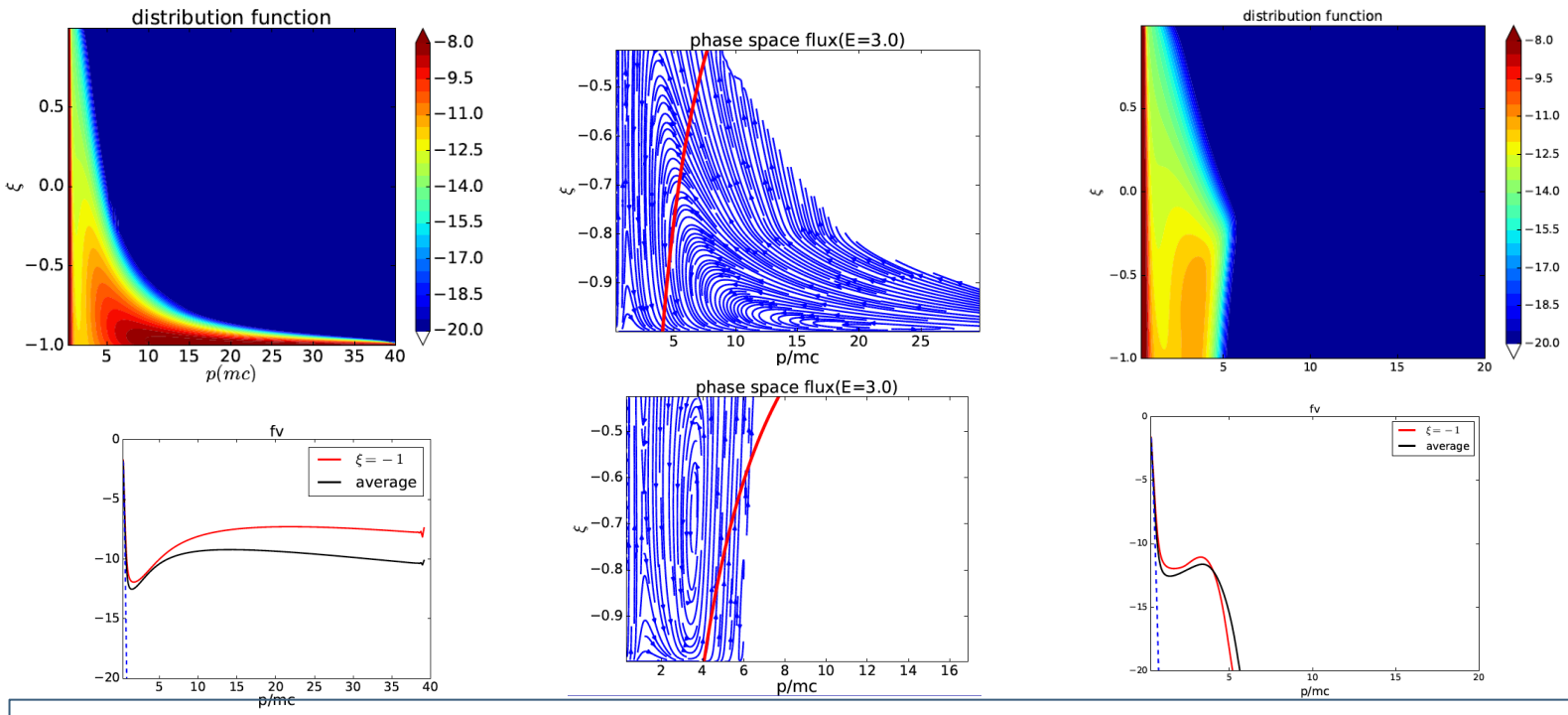
Runaway control: externally injected waves

- If runaway current is unavoidable, mitigation can be achieved by limiting the runaway energy via a “surgery” of runaway vortex by externally injected waves
  - Underlying principle: enhanced pitch-angle scattering reshape runaway vortex
  - We will use whistler wave at normal Doppler resonance

No waves

$$\omega_{kr} - k_{\parallel} v_{\parallel} - \gamma^{-1} = 0$$

With waves



Z. Guo, C.J. McDevitt, and X.Z. Tang, “Control of runaway electron energy using externally injected whistler waves,” Physics of Plasmas 25 (3), 032504 (2018).

Outline: SCREAM highlights in theory and simulation of REs

- Runaway electron generation
  - Full orbit simulations of runaway electrons with KORC
  - The backward Monte Carlo and Adjoint methods for runaway probability
  - The lifetime of runaways
  - Runaway vortex
- Thermal quenches and magnetic surface breakup
  - Reduced modeling of VDEs
  - Disruptions and RE Modeling with NIMROD and RE Orbit Modeling
- Mitigation via impurity injection
  - In MHD simulations of MGI and SPI with RE tracers
  - Theoretical efforts to better understand experiments
- Whistler wave scattering of runaway electrons
  - Explaining experimental observations of spontatneous onset
  - Exploring the use of wave launching to mitigate REs
- Advanced Vlasov-Fokker-Planck solvers
  - Conservative relativistic Fokker-Planck solvers
  - Conservative adaptive algorithms for the Landau collision integral
  - Conservative Hamiltonian Vlasov integrators
- Highlights of future directions

Conservative solvers for RE kinetics are key to future research

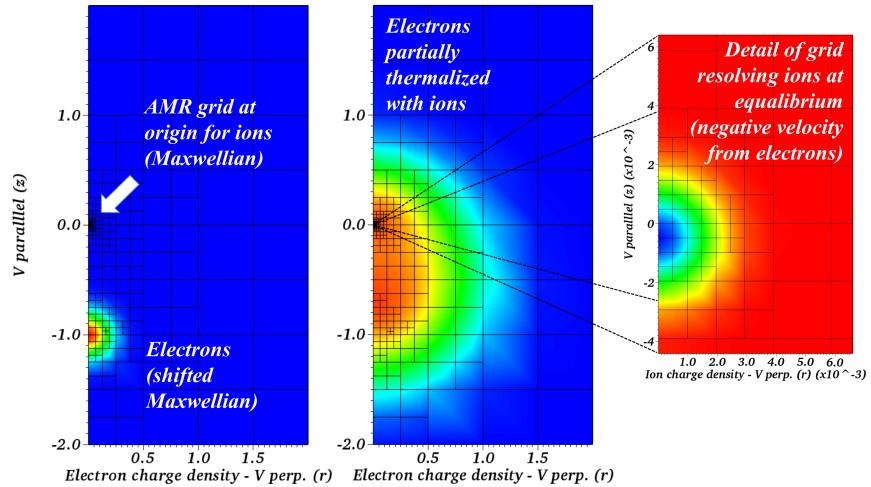
- Due to the need for long timescale simulations of RE generation and dynamics, eventually coupled with MHD, truly conservative solver methods for electron kinetics are a high priority development focus of the SCREAM project

- Conservative methods being explored in both continuum and particle based formulations

Fully Conservative, Adaptive, Discretization of Landau Collision Integral for Emerging Architectures in PETSc

Scientific Achievement

The Landau collision integral is the gold standard for integrating many body dynamics into the standard phase space model of fusion plasmas – Vlasov's equation. In collaboration with plasma physicists at PPPL, LBNL computational scientists have developed the first fully conservative, adaptive (finite element) discretization of the Landau collision integral, optimized for the the 2nd Generation Intel Xeon Phi (``Knights Landing'') processor



This graphic illustrates an electron beam thermalizing with ions in phase space with axisymmetric geometry

Significance and Impact

Vlasov's equation with a Landau collision operator is the fundamentally the best model for fusion plasmas and this work contributes the best (full conservative, high order accurate, adaptive) discretization of Landau to date. Provides step toward full Vlasov-Boltzmann model and discretization is computationally efficient, accurate & fully conservative

Research Details

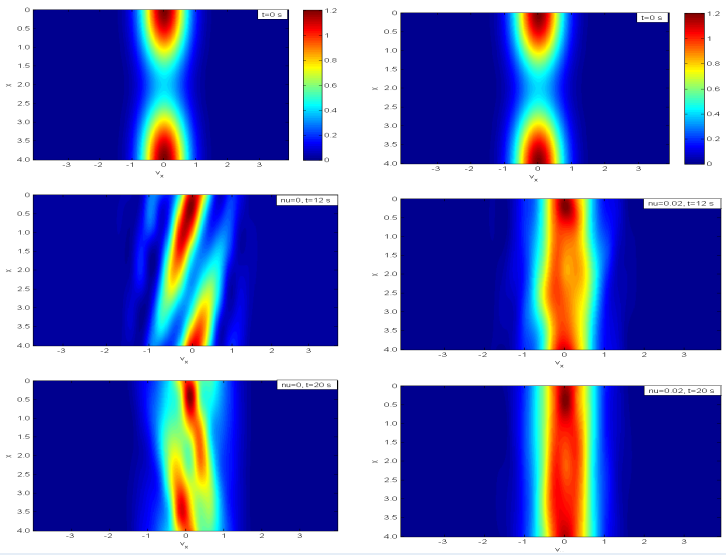
- The Landau collision integral is an accurate model for the small-angle dominated Coulomb collisions in fusion plasmas. We develop a high order accurate, fully conservative, finite element discretization of the nonlinear multi-species Landau integral with adaptive mesh refinement using the PETSc library's (www.mcs.anl.gov/petsc) Solver Integrated Tree-based Adaptive Refinement (SITAR) infrastructure

M. F. Adams, E. Hirvijoki, *Physics of Plasmas, 2017*

M. F. Adams, E. Hirvijoki, M. G. Knepley, J. Brown, T. Isaac, and R. Mills, *SIAM J. Sci. Comp., 2017*

Conservative Scheme for Vlasov Poisson Landau modeling collisional plasmas

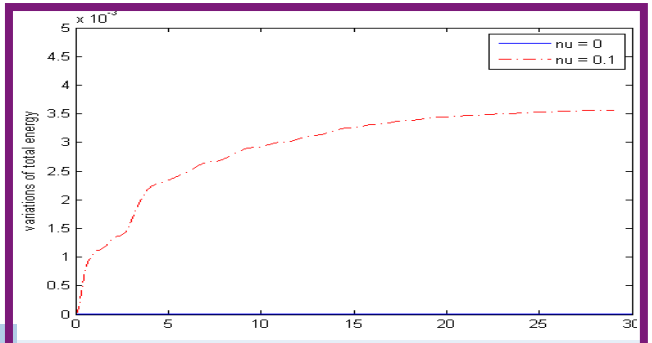
Energy conservative schemes for, both, Vlasov-Poisson-Landau systems by means of hybrid conservative Lagrangian schemes for the non-linear Landau operator and for DG schemes for Vlasov-Poisson systems



nodes	cores	wall clock time (s)
1	12	1228.18
2	24	637.522
4	48	307.125
8	96	154.385
16	192	80.6144
32	384	41.314

HPC: Wall clock time for a single time step for a typical Landau damping problem TACC cluster, 2016

PDF countors evolution: **mfp** ν = 0(left), ν = 0.1(right)
Amplitude=0.5,T=0.25,k=$2\pi/4$ and L_v =4.
Mesh: Nx =48, Nv =32. NlogN solver on Fourier nodes $N_v^3=24^3$



Total (kinetic+potential) energy rel. error: two-stream flow model
mfp: ν = 0(blue), ν = 0.1(red)

C. Zhang and I.M.Gamba, A Conservative Scheme for Vlasov Poisson Landau modeling collisional plasmas, arXiv:1605.05787v2, J. Comput. Physics, 2017.

Outline: SCREAM highlights in theory and simulation of REs

- Runaway electron generation
  - Full orbit simulations of runaway electrons with KORC
  - The backward Monte Carlo and Adjoint methods for runaway probability
  - The lifetime of runaways
  - Runaway vortex
- Thermal quenches and magnetic surface breakup
  - Reduced modeling of VDEs
  - Disruptions and RE Modeling with NIMROD and RE Orbit Modeling
- Mitigation via impurity injection
  - In MHD simulations of MGI and SPI with RE tracers
  - Theoretical efforts to better understand experiments
- Whistler wave scattering of runaway electrons
  - Explaining experimental observations of spontatneous onset
  - Exploring the use of wave launching to mitigate REs
- Advanced Vlasov-Fokker-Planck solvers
  - Conservative relativistic Fokker-Planck solvers
  - Conservative adaptive algorithms for the Landau collision integral
  - Conservative Hamiltonian Vlasov integrators
- Highlights of future directions

Numerous publications over 2016-18 are indicative of significant progress in RE physics

- A range of computational, theoretical and experimental analysis appears in publications – a broad spectrum
- At least 37 journal articles published with team member authorship since ‘16 initiation, including:
  - 3 PRLs involving DIII-D experimental analysis (more in review)
  - New physics mechanisms identified which are directly relevant to the goals of SCREAM
    - Whistler scattering effects identified in experimental data
      - Critical electric field and mechanisms for mitigation strongly affected
    - Significant progress in understanding confinement, transport and energetics of relativistic electrons
    - Multiple new mitigation ideas being explored, including wave launching

Future Plans for SCREAM in Brief

- Phase space dynamics
  - Investigate physics of RE generation and evolution with wave particle interaction
  - Application of wave particle interaction to passive and active control
- Test particle simulation in MHD
  - Bring the capabilities of M3D-C1 into the research plan
  - Include MHD fluctuations and continue to investigate collisions including knock-on
  - Study RE seed generation during disruption simulations
  - Study the decay rate of mature runaway beams
- Self-consistent full kinetic and hybrid modeling
  - Development of full orbit, drift kinetic and bounce-averaged relativistic Fokker-Planck solvers (2D-2V up to 3X-3V)

Progress Advancing: FES theory and modeling with numerical simulation facilitated by ASCR applied mathematics

Full range of team contributions

- Vlasov Fokker-Planck Discrete Continuum Modeling of Runaways
- Applied Math / Solver Methods for HPC
- Coupling Algorithms for Kinetic / Fluid Hybrid Simulations
- Monte Carlo / PIC Simulations of Runaways
- MHD Simulation of disruptive instabilities and thermal collapse
- Theoretical Analyses and Scoping Studies for Guidance

Goal: Kinetic Runaway Modeling of Avoidance and Mitigation Techniques coupled to MHD and WDM