Recent advances in the theory and simulation of runaway electrons in the SCREAM SciDAC

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On behalf of the SCREAM Team (scream.pppl.gov)

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Outline: SCREAM highlights in theory and simulation of runaway electrons

- The physics of RE generation and disruption dynamics
- Wave particle interactions of REs
- Runaway electron generation, advancing to 3D+2V simulations
- Runaway confinement in 3D, disruption simulations, and mitigation via impurity injection
- Putting it all together: Future directions toward WDM
  - developing solvers for widespread deployment
  - integrated simulations and predictive modeling

Runaway Electron mitigation is a critical issue in tokamak fusion energy science

As most electrons get cooled due to collisions, electric field in disruptions can drive remnant of hot electrons from keV to MeV which become runaway electrons.

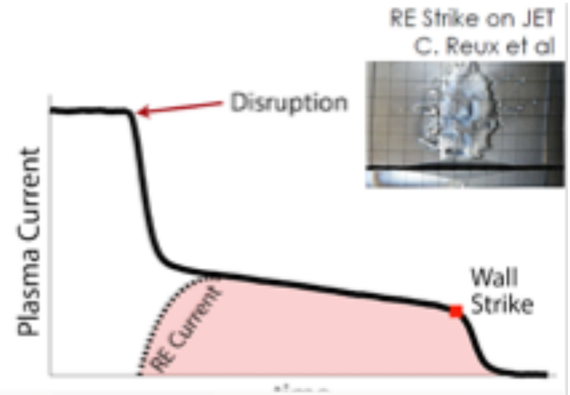
Knock-on collision of high energy electron with thermal electron can lead to avalanche growth of REs.

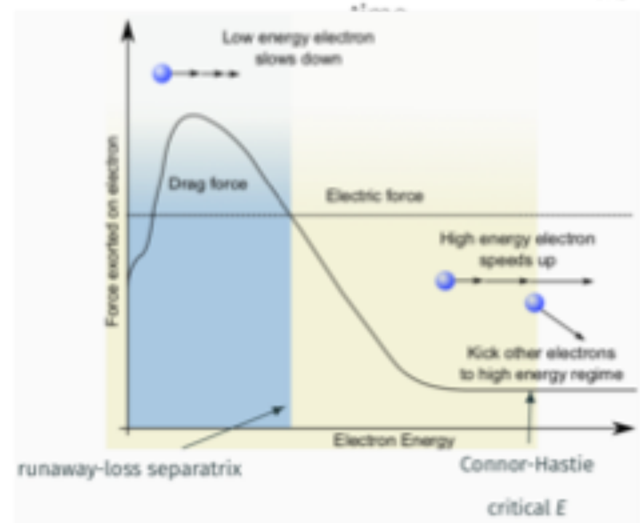
RE beam can strike the first wall during final loss and cause damage to the device.

In an ITER disruption, a large population of energetic runaway electrons can be generated due to the strong inductive E field. Limited opportunity to study empirically in present day devices: different regimes than ITER.

Disruption may be unavoidable, so it is important to mitigate RE beam: suppress generation, limit energy, diffuse to the edge.

Simulation Center for Runaway Electron Avoidance and Mitigation
A theoretical predictive model is essential, understanding must advance rapidly now.





Recent theoretical results indicate RE problem will be a severe threat

Poloidal flux content at which runaway becomes dangerous, Ψp, is proportional to γ_{ef}

$$\gamma_{ef} \equiv \frac{\text{electron collision rate at critical energy for runaway}}{\text{collision rate of relativistic with background electrons}} \approx 2.39\,\Lambda$$

Ψp is also proportional ℓ_f

$$\ell_f \equiv \log_{10} \frac{\text{relativistic electron density required to carry current}}{\text{number density of seed electrons}}$$

The residual pre-thermal-quench Maxwellian tail is the most important seed if the timescale for the thermal quench and for the time magnetic surfaces are open is short enough ~< 10 ms.

The steady-state seed due to either tritium decay or to Compton scattering can make runaway a major issue in the nuclear phase of ITER even when there is no problem in the non-nuclear phase. The rate Compton scattering produces seed electrons is proportional to number of background electrons (bound and free). Particle injection may make runaway problem much worse on ITER; can even make γ_{ef} much smaller.

A.H. Boozer, PPCF 61, 024002 (2019)

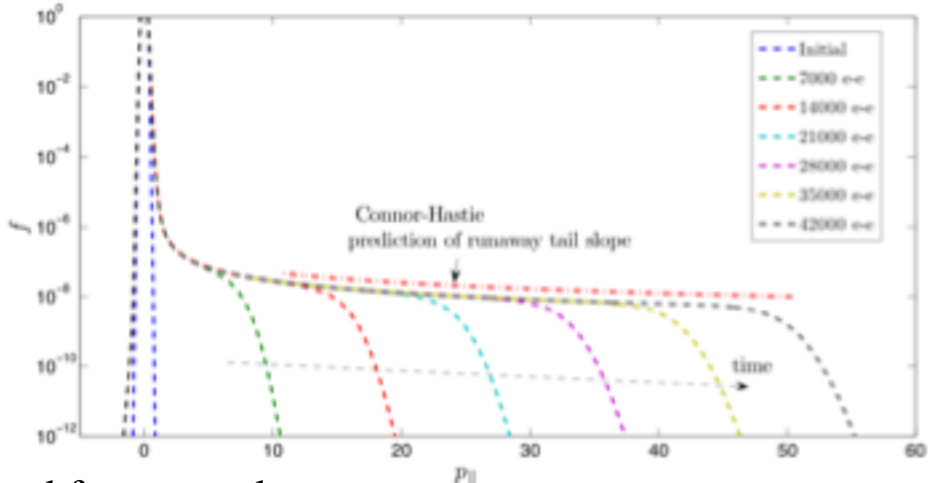
A fully implicit, optimal, massively parallel and scalable, conservative, nonlinear relativistic Fokker-Planck solver developed for runaway electrons

Run-away tail generation – Connor-Hastie comparison

$$f = A\frac{1}{p_{\|}}\exp - \frac{(\alpha+1){p_{\perp}}^2}{2(1+Z)p_{\|}} \qquad \alpha = \frac{E}{E_c}$$

Connor-Hastie asymptotic limit for the tail Distribution (red dashed line)

Time evolution of the electron distribution $E/E_c = 2.25, \Theta = 0.01, Z = 1$



Capturing small amplitude tails require accurate positive-preserving schemes

Extensive verification to be reported in JCP: conservative properties, conductivity(E), tail and distribution dynamics

Current and future work:

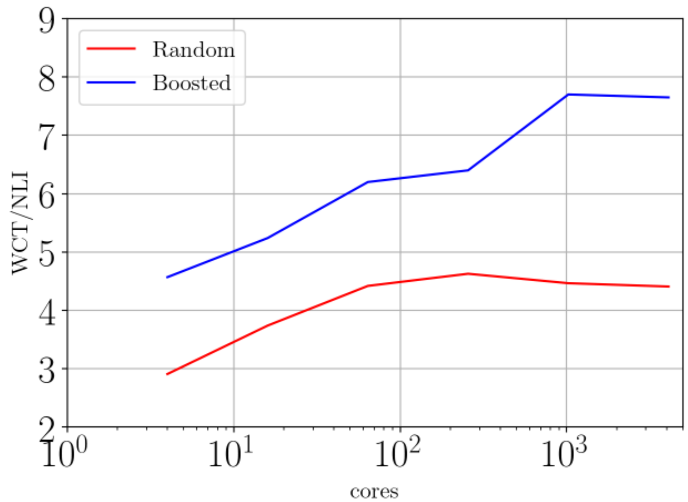
- Dynamics along drift orbits (1D-2P) using asymptotic-preserving semi-Lagrangian methods
- Knock-on (large angle) collisions
- Coupling with ion physics

D. Daniel, W. Taitano, and L. Chacon, submitted JCP 2019

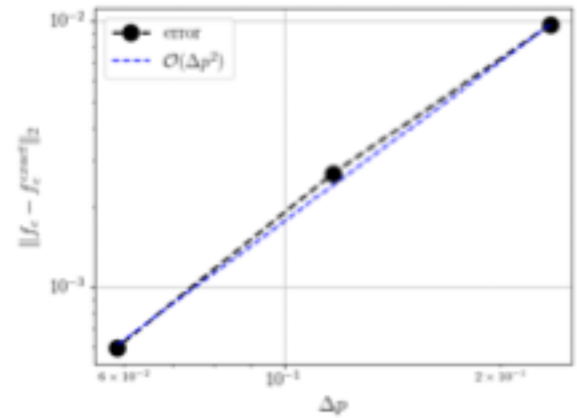
Parallel scalability and temporal accuracy verified

Parallel and algorithmic scalability demonstrated up to 4096 cores

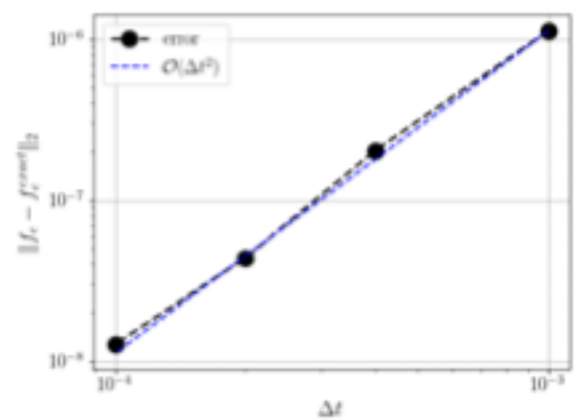
Wall clock time per nonlinear iteration



Spatial second-order accuracy



Temporal second-order accuracy



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Continuum Relativistic Electron Kinetics being developed to study RE physics, including saturation and control

- Physics model: relativistic Fokker-Plank-Boltzmann equation + radiation damping + atomic processes
- Grid-based method (0D-2V)
  - LAPS-RFP continuum module (Guo et al., PoP, 2019)
- Solvers have been used to elucidate runaway electron energy saturation mechanism ➔ runaway vortex (Guo et al., PPCF, 2018)
  - Presence of runaway vortex provides a retainer for secondary runaways to accumulate
  - Disappearance of runaway vortex linked to avalanche threshold (McDevitt et al., PPCF, 2018)
- Resonant wave-particle scattering via externally injected whistler waves, can manipulate the runaway vortex by cutting off the high energy part (Guo et al., PoP, 2018)
  - Means of runaway energy control via phase space engineering

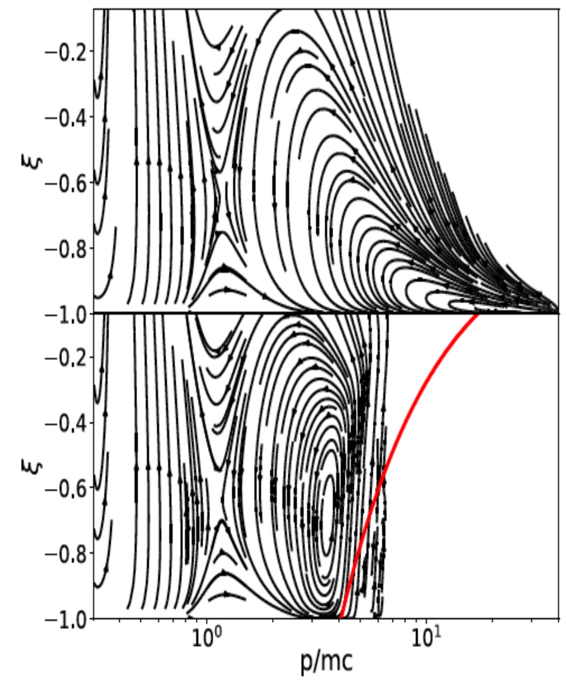


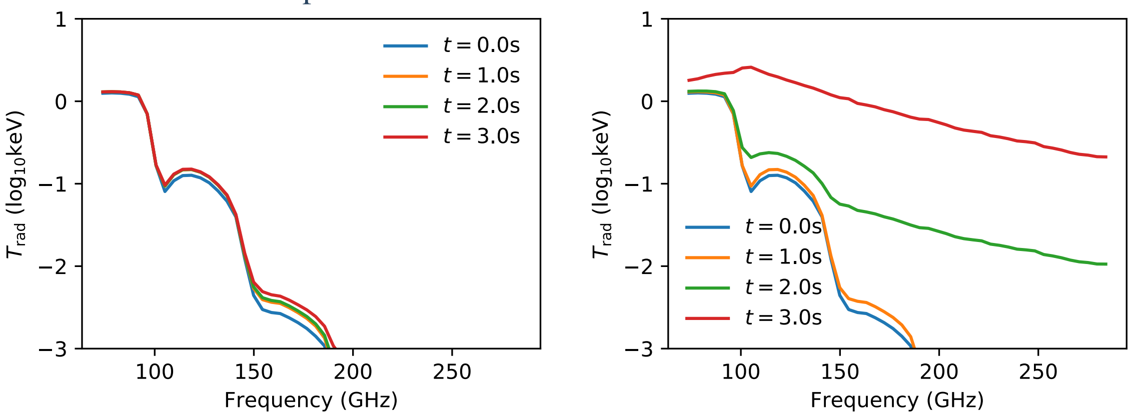
FIG. 4. The primary electron energy and pitch-angle fluxes $(p^2\Gamma_p/f, p\Gamma_\xi/f)$ in momentum space. $p_O \approx 20$ without whistler waves, while $p_O \approx 3.5$ with injected whistler waves, which is a factor of 5.7 lower. The X point is little changed in both cases. The red curve in the bottom plot labels the resonance condition at the peak of the applied Gaussian wave spectrum, Eq. (15). The design freedom in placing this resonance in (p, ξ) space allows precise control of the runaway vortex and hence the runaway energy.

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

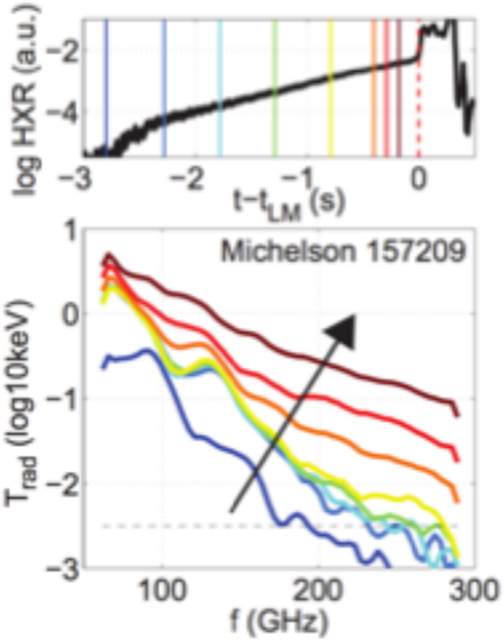
Key result: whistler scattering is largely responsible for the dynamic growth of energy spectrum observed in QRE experiments

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

Simulated ECE spectrum



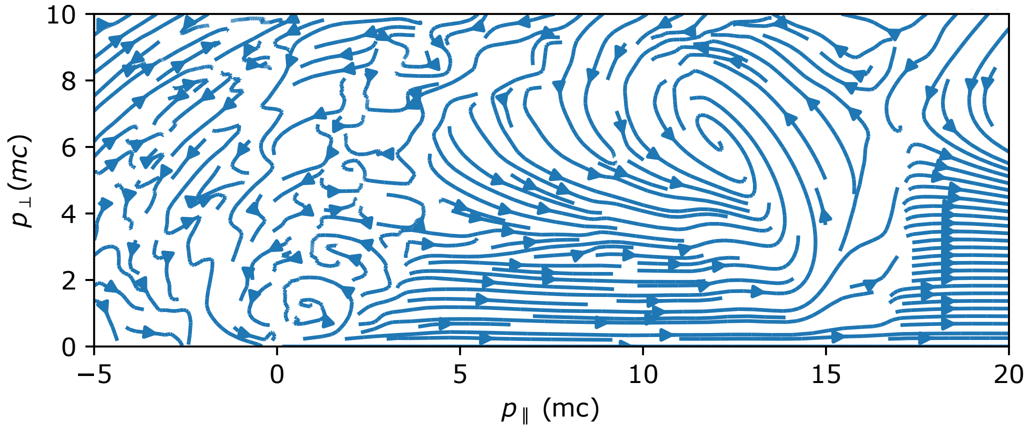
ECE Spectrum evolution during RE growth in DIII-D

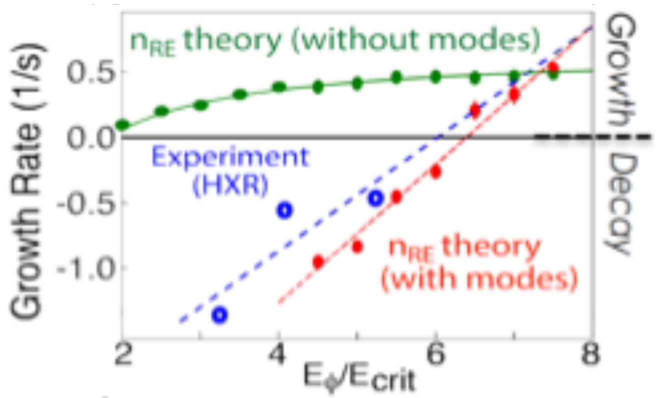


Now clear that whistler scattering is critical physics needed to interpret many runaway electron experiments

Chang Liu, et al arXiv:1803.09897, Nucl. Fusion (2018).

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





Experimental measurements of critical electric field for runaway nave 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 important effect in ITER.

New developments:

- bounce-average model for RE kinetic equation. -> toroidal effects & Alfven Eigenmodes
- collision operator includes partially-screening effect (L. Hesslow PRL 2017)

C. Liu et al, arXiv:1801.01827, Phys. Rev. Lett. 120, 265001 (2018)

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Avalanche Amplification of a Seed Runaway Electron Population

- Number of amplifications of a “seed” population can be estimated by:

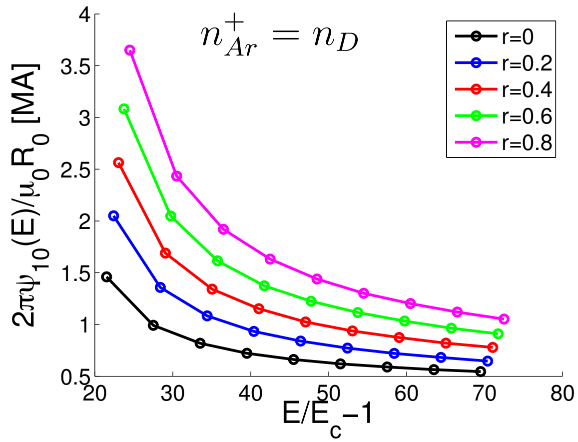
$$N_{10} = \frac{1}{\ln 10}\int_{t_i}^{t_f} dt\gamma_{av} \approx \frac{1}{\ln 10}\frac{\gamma_0}{E_c R_0}\int_{t_i}^{t_f} dt\frac{\partial\psi}{\partial t} = \frac{\Delta\psi}{\psi_{10}}$$

$$\boldsymbol{\gamma}_{av} = \boldsymbol{\gamma}_0\left(\frac{E}{E_c} - 1\right)$$

- Without impurities: $2\pi\psi_{10}/\mu_0 R_0 \lesssim 1\ \mathrm{MA}$ [Rosenbluth-Putvinski 1997, Boozer 2018]
  - Implies a seed population in ITER (I_p=15 MA) can be amplified by 10^{15}!
  - Suggests that “seed” electrons arising from Tritium or Compton scattering during the DT campaign of ITER cannot be ignored
- In a weakly ionized plasma [McDevitt et al. PPCF 2019]:
  - An effective ψ_{10} can be derived that has a strong dependence on the electric field strength
  - Near threshold ψ_{10} significantly increased
  - Above threshold ψ_{10} decreases:

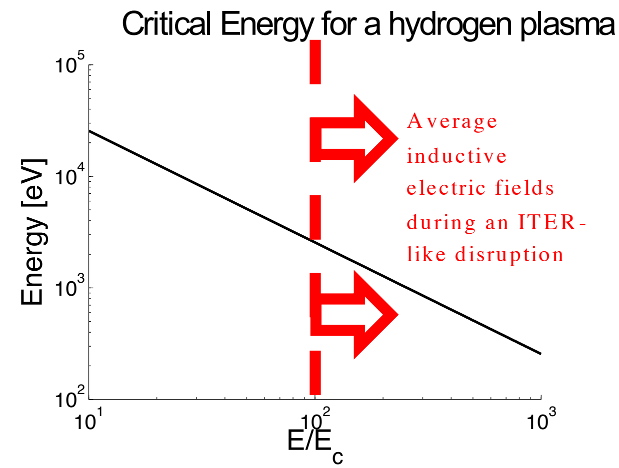
$$2\pi\psi_{10}/\mu_0 R_0 \approx 0.5\ \mathrm{MA}$$

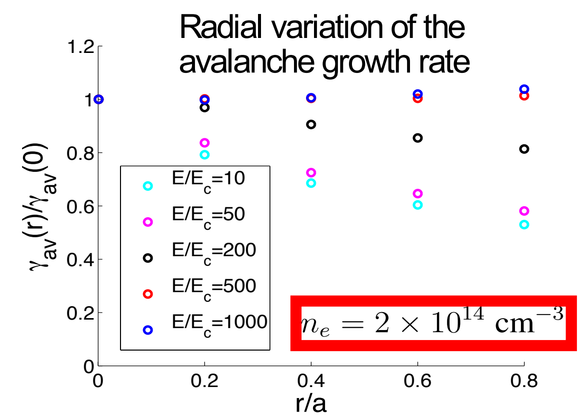
  - Implies potential 10^{30} seed amplification in ITER!
  - ψ_{10} increases significantly at larger radii for modest electric fields



Runaway Generation Processes in Tokamak Plasmas for Large Inductive Electric Fields

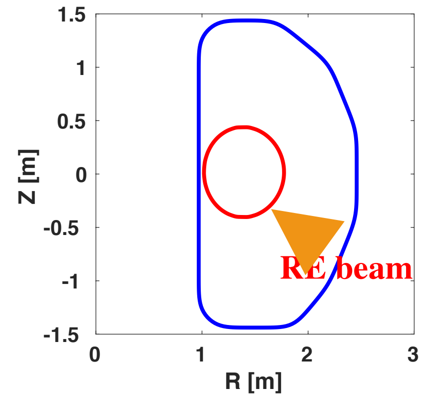
- Previous work on how toroidal geometry impacts runaway generation largely focused on electron trapping
  - →Implies a reduction of runaway generation as the minor radius is increased
- For large electric fields the critical energy for an electron to run away can decrease to several hundred eV
  - Electrons at these modest energies are often characterized by $\nu_* \gtrsim 1$
  - Electron trapping effects largely negated at these energies
  - Results in the avalanche growth rate asymptoting to a nearly constant value as the minor radius is varied [McDevitt et al., submitted EPL, 2019

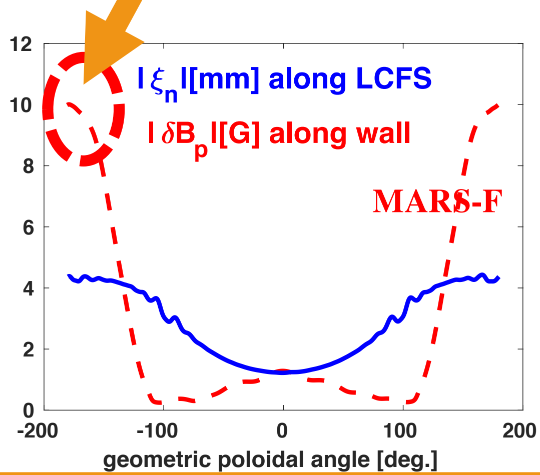


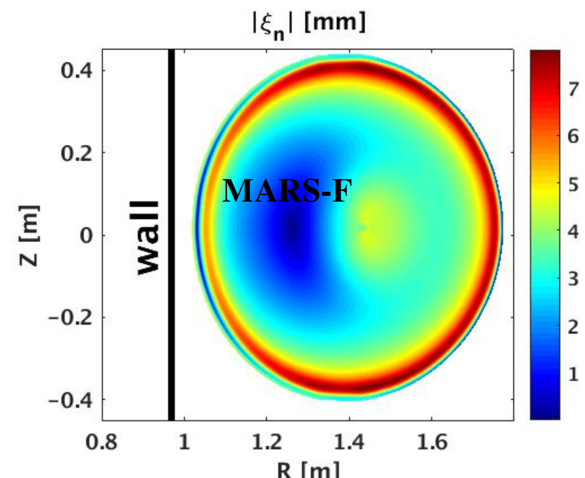


Work is in progress to study MHD instability induced loss of post-disruption high current RE beam in DIII-D

- Shot 177040@1025 ms: B_0=2.13 T, I_p=770 kA, q_a~2
- MARS-F computes an unstable n=1 resistive kink mode (REK) with both internal & external structures
- New RE drift orbit module implemented into MARS-F
- Mode amplitude defined as δB_p at HFS wall location
- Experiments: large RE loss with δB_p ~ 10-100 G [Paz-Soldan PPCF19]; Modeling: scan amplitude while keeping n=1 REK eigenmode structure

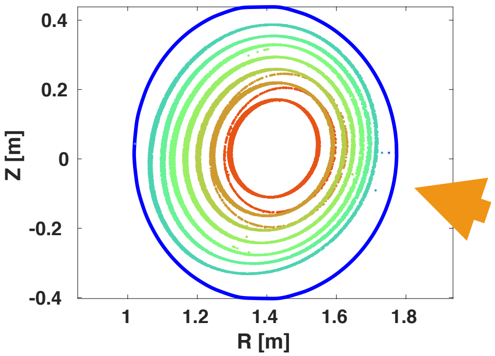






1 kG resistive kink perturbation leads to full RE loss, consistent with DIII-D experiment

δB_p=50G

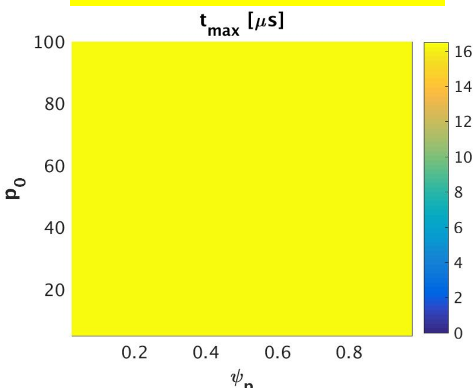


lost RE

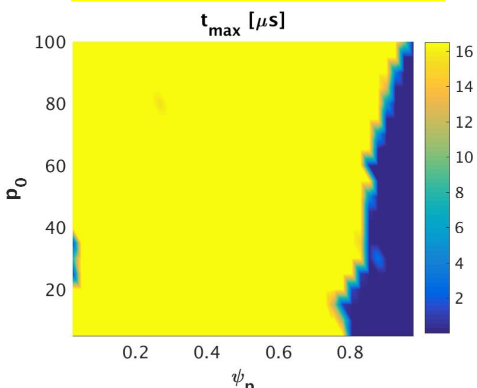
- λ_0=RE pitch angle at t=0, fixed at 0.1
- Vary initial radial location of REs & initial particle energy

- More loss at lower energy
- Essentially full loss as 103 G level field perturbation
- Key loss mechanism: prompt drift orbit loss

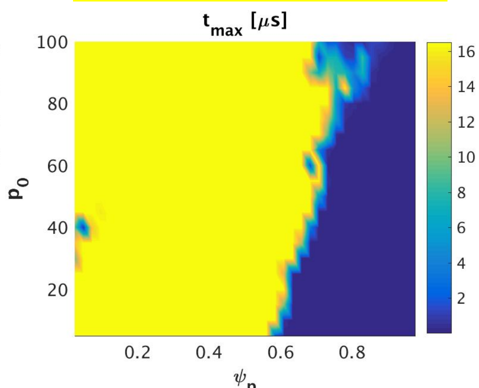
δB_p=0G



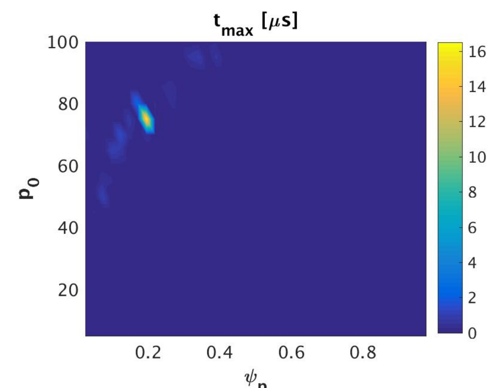
δB_p=100G



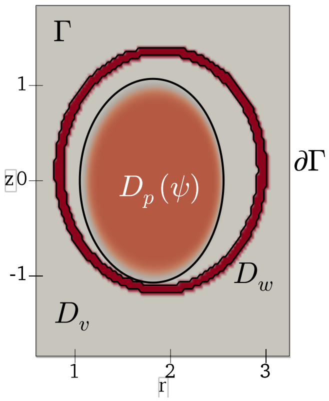
δB_p=200G



δB_p=10^3G



FORCE-FREE MOTION OF A COLD PLASMA DURING THE CURRENT QUENCH



Basic equations

Force-free constraint

$$\boxed{r^2\nabla\cdot\left(\frac{\nabla\psi}{r^2}\right)=-I\frac{dI}{d\psi}.}$$

Magnetic field diffusion

$$\frac{\partial\psi}{\partial t}=D(\psi)r^2\nabla\cdot\left(\frac{\nabla\psi}{r^2}\right)-\boldsymbol{V}\cdot\nabla\psi;$$

$$\frac{\partial I}{\partial t}=r^2\nabla\cdot\left(\frac{D(\psi)\nabla I-\boldsymbol{V}I}{r^2}\right).$$

The plasma velocity arises as a consequence of the force-free constraint

Conclusions

- Dissipation of the magnetic flux forces the plasma to go through a sequence of the force-free states [1, 2];
- $(\boldsymbol{n}_w\cdot\boldsymbol{V})$ does not vanish at the wall [2];
- The poloidal and toroidal wall currents give comparable contribution to the force acting on the wall [2];
- The frozen-in condition breaks down during the cold VDE [2];
- An effort to decrease the current decay time by increasing the amount of injected impurities may change the current carriers from bulk electrons to runaway electrons but will not decrease the plasma current value when the plasma touches the wall [1, 2].

[1] D. I. Kiramov and B. N. Breizman, Physics of Plasmas **25**, 092501 (2018).

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

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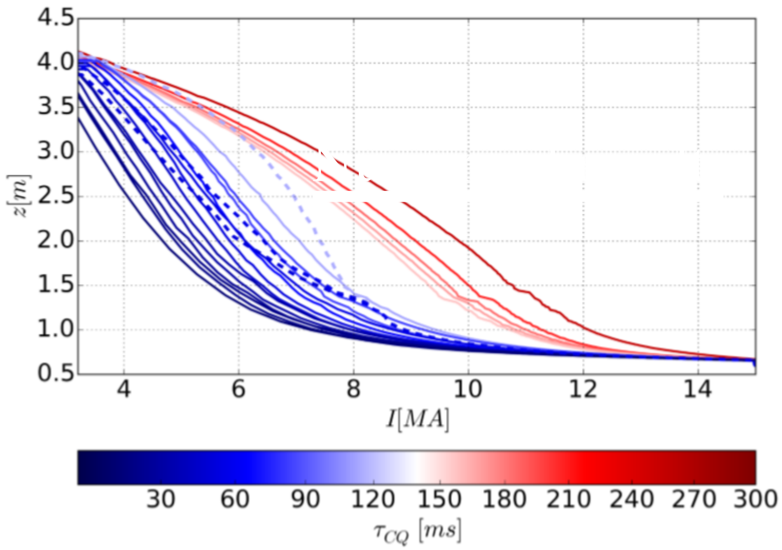


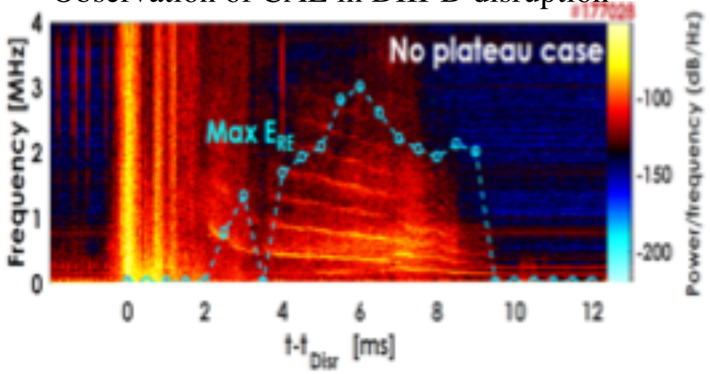
DINA code results. The plasma vertical position as a function of the plasma current. Colors represent the current quench duration. The curves converge to the ideal wall limit as the current quench time decreases.

- In the ideal wall limit, the vertical coordinate of the plasma column has a universal monotonic dependence on the toroidal plasma current;
- Numerical simulations confirm the theoretical predictions of [1,2];
- An effort to decrease the current decay time by increasing the amount of injected impurities will not decrease the plasma current touching the wall.

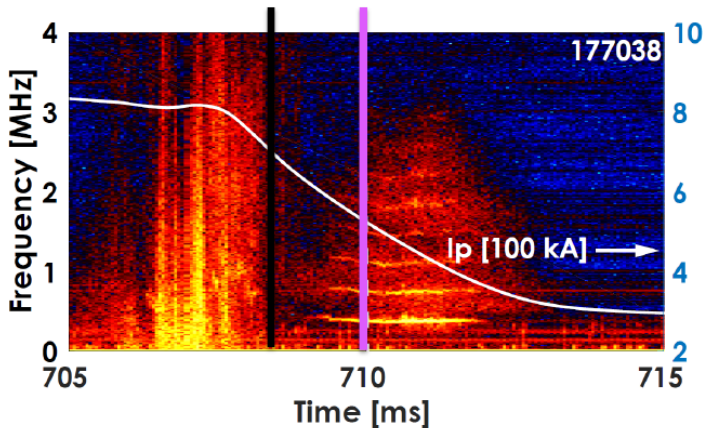
Using new quasilinear code to study excitation of compressional Alfven eigenmode (CAE) excited in DIII-D disruptions

- CAE has been directly observed in DIII-D experiments and is connected to the dissipation of RE current.
- Calculate the mode structure and the growth rate with quasilinear code, confirming that the mode can be excited by runaway electrons in disruption scenario.
- Excitation of CAE can lead to spatial diffusion of REs, which is a promising candidate for alternative RE mitigation strategies.
    - Collaboration with DIII-D experimentalists (C. Paz-Soldan) and RF SciDAC group (N. Bertelli) to explore this new approach.

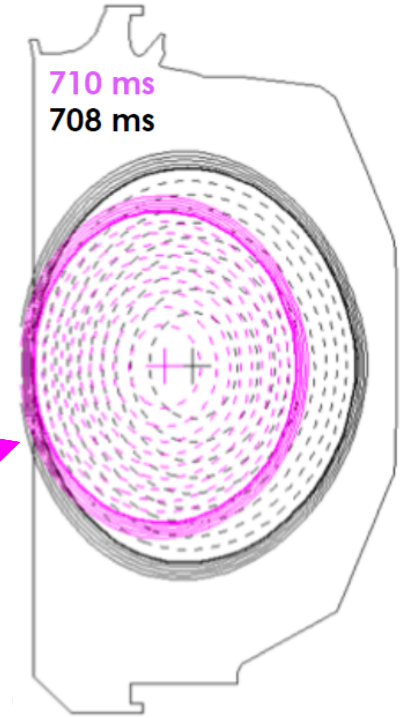
Observation of CAE in DIII-D disruption



AORSA fast wave simulations for RE-driven CAEs in DIII-D post-TQ phase of a disruption



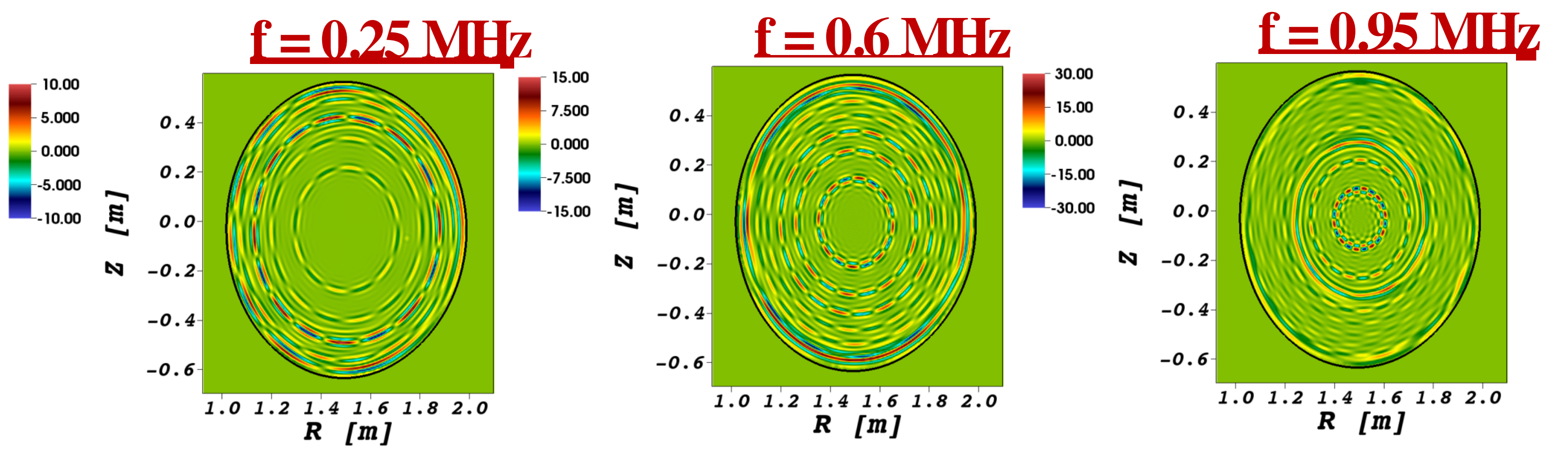
- Frequency scan for a DIII-D scenario @ 710 ms
  - 0.25 – 1 MHz
  - $n_\phi = 1$
- n_e = CONST. = 4.8×10^{19} m^{-3}
- T_e = CONST. = 2 eV (cold plasma)
- Plasma species: electron and D



Collaboration between SCREAM and RF SciDAC for quantitative details on mode structure and growth rate for RE interaction

What is the mode structure of the CAEs excited?

- Full wave AORSA simulations
- Assuming antenna on the LCFS
- Re($E_{||}$) shown below for three frequency values

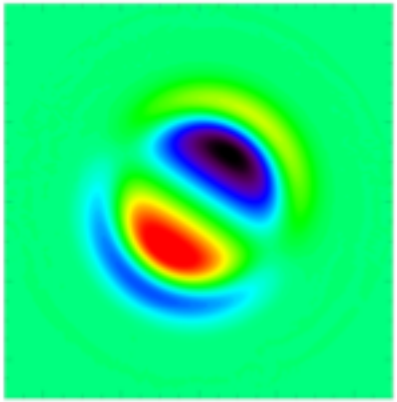


Fluid model of runaway electron in M3D-C1

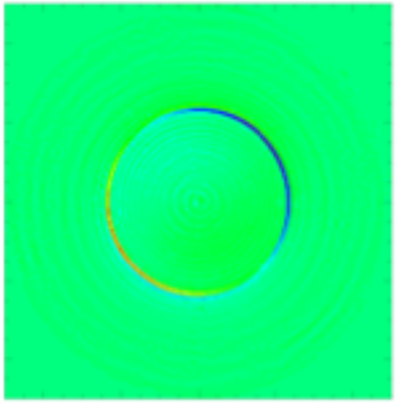
- Compared to particle-based model, the fluid model is easier to implement in a MHD code and less expensive for computation.
  - Similar mode has been successfully implemented in EXTREM code (Japan), and is now being developed in JOREK (Europe) and NIMROD
- Goal: study the impact of RE current on MHD stabilities.
- After implementing RE generation source term, conduct integrated simulation for disruptions including pellet injection, RE generation and MHD instabilities

Collaboration with CTTS SciDAC.

Perturbed current of (1,1) mode
From M3D-C[1] without RE current

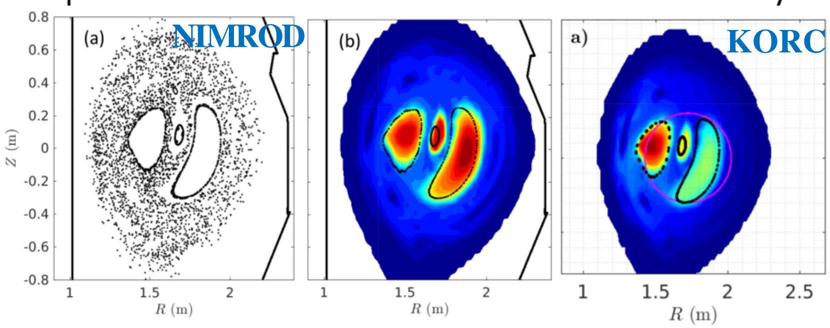


Perturbed current of (1,1) mode
with RE current



3D full-orbit spatially dependent effects KORC computations uncover critical physics

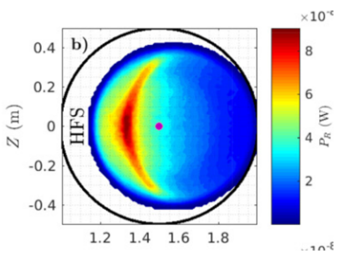
Spatial dependence of synchrotron emission in the presence of 3D fields with islands and stochasticity



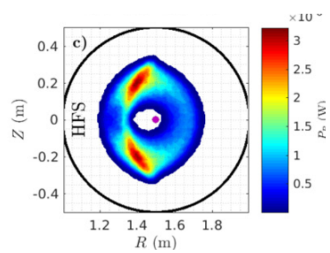
3D Stochastic magnetic field Poincare plot

RE particle distribution

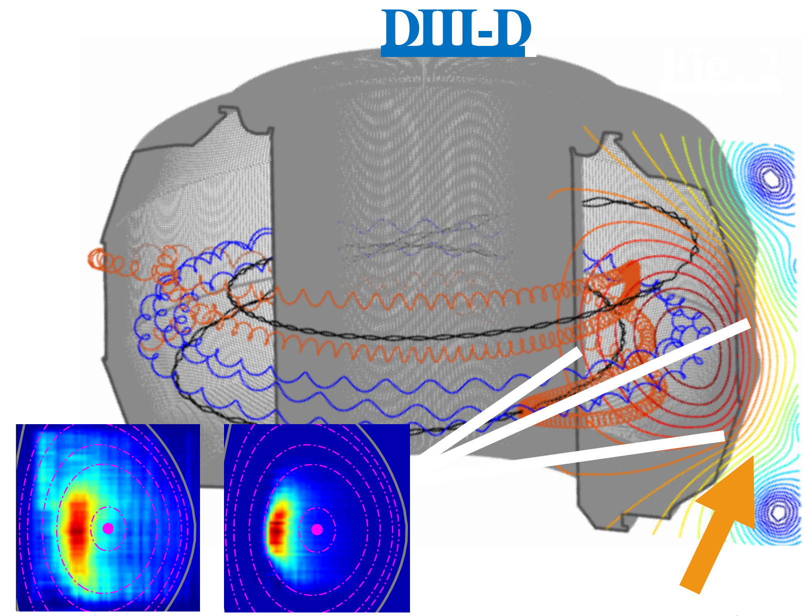
Synchrotron emission spatial distribution



Passing RE



Trapped RE



DIII-D measured synchrotron emission

EFIT magnetic field reconstruction

Model validation

Encouraging steps toward fully coupled particle simulations in KORC and simulations of disruptions in MHD (M3D-C1 and/or NIMROD)

del-Castillo-Negrete, Carbajal, Spong and Izzo, Phys. Plasmas **25**, 056104 (2018).
Carbajal and del-Castillo-Negrete. PPCF **59**, 124001 (2017); Carbajal, et.al., IAEA (2018).

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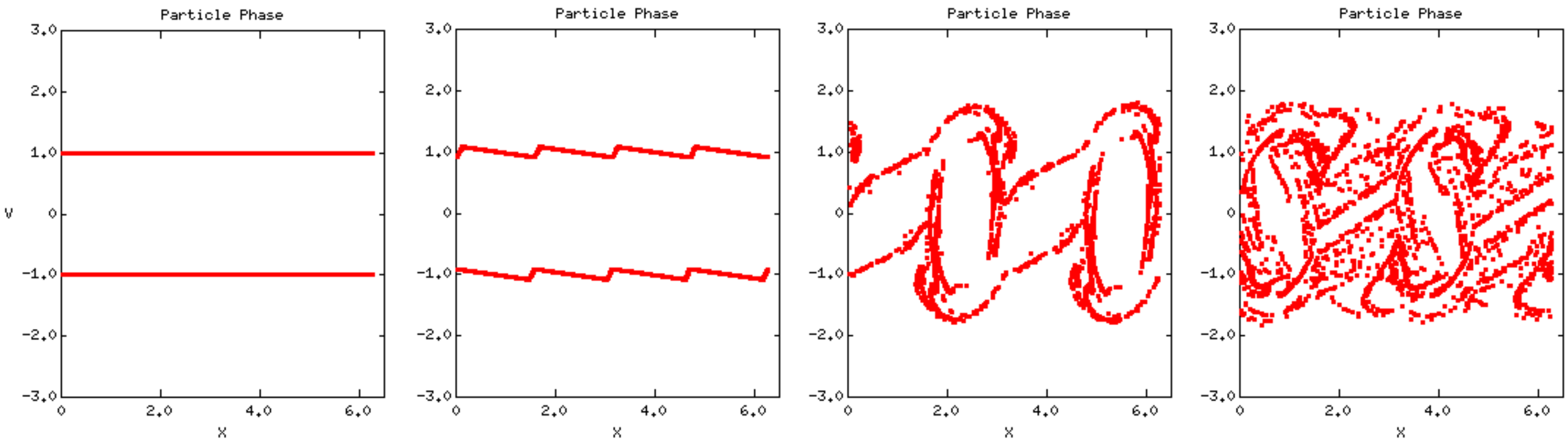
Structure Preserving Geometric Electro-Magnetic Particle-in-Cell (GEMPIC) methods deployed in PETSc

- Advanced, structure preserving (SP) PIC discretizations of Vlasov-Maxwell-Fokker-Plank developed in GEMPIC method
  - M. Kraus, et al.
- PETSc (Portable Extensible Toolkit for Scientific Computing) widely used package of numerical methods for HPC modeling
- LBNL and U. Buffalo developing finite element version of GEMPIC and deploying its components in PETSc:

  1. Symplectic Timestepping
  2. Conservative Projection Operator
  3. Continuous E-Field Poisson solvers
  4. Collision Operator
  5. Entropic Integrators

Electrostatic Vlasov Example: Two Stream Instability

- Two-Stream instability represents a well known problem presented in Birdsal-Langdon
- Two opposing beams of same-species particles overlaid in 1D with opposing drift velocities

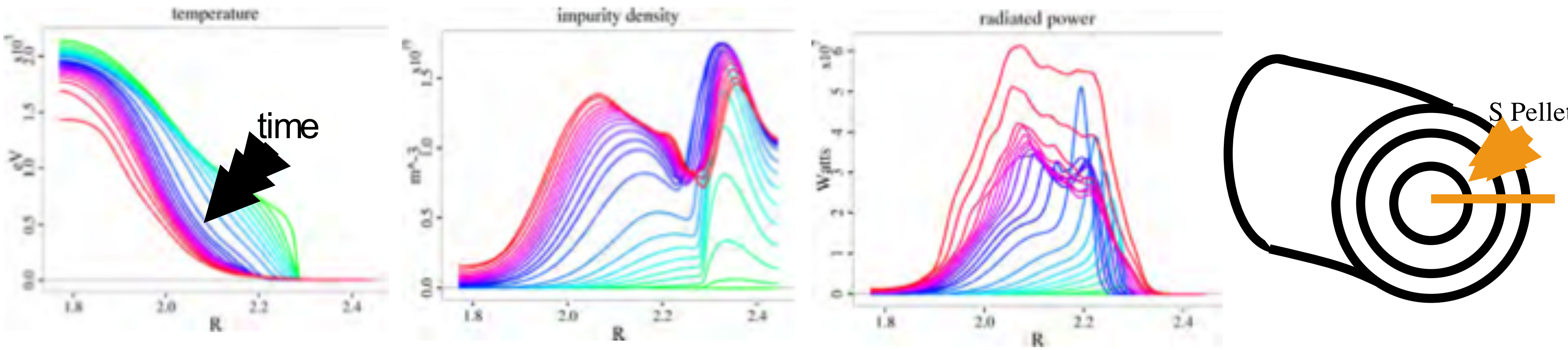


<u>GEMPIC – The Point:</u>

Develop full structure preserving integrators with conservation to machine precision

Deploy methods (eg, time integrators, Particle-cell mapping, Fokker-Planck) in PETSc for use in Vlasov PIC applications

CQL3D Coupled to NIMROD Profiles From Shattered Pellet Simulation



Plasma profiles at the midplane major R coord., from NIMROD simulation of shattered pellet injection in DIII-D.

NIMROD provides data on time-dependent radial profiles of T_e, T_i, n_e, current density j.

These profiles are adapted to CQL3D radial grid

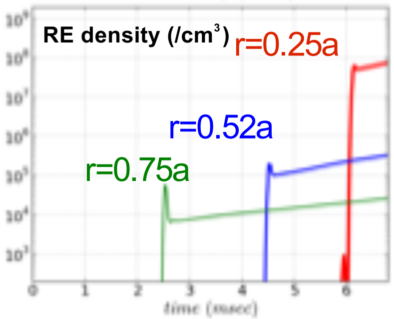
Toroidal elec field E_{tor} is evaluated from plasma current and Spitzer resistivity.

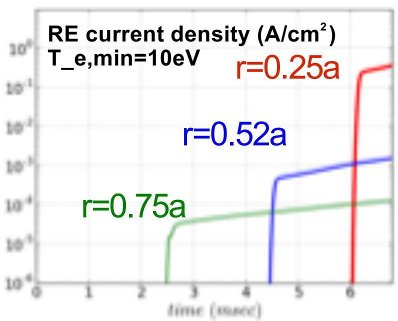
CQL3D calculates time-dep RE density, RE current density with given $E_{tor}(r,t)$

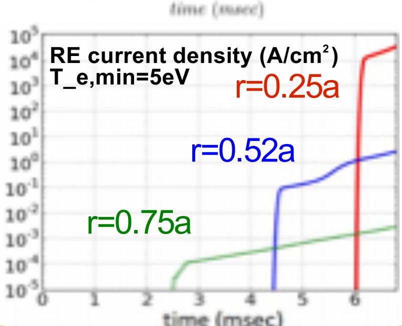
Currently under development: pass $J_{\parallel}$ (and $f_{RE}(z)$) to NIMROD, implement in hybrid kinetic-MHD module

B. Harvey, C.C. Kim, L. Lao 2019

CQL3D Calculates RE Density and Current Using NIMROD Profiles







Extreme sensitivity to last few eV in Te drop

CQL3D calculations of RE density and current resulting from NIMROD t-dependent profiles for the case of shattered pellet deposition, giving a thermal quench and indicating knockon avalanche.

.REs start from plasma edge (green) where Te drops to 10eV or 5eV sooner than in plasma center (red), as the pellet stream traverses the plasma.

.There is sufficient "hot tail runaway" to begin a RE avalanche.

.E/E_{crit} is ~500 across most of plasma, giving knockon growth rate ~0.5/msec.

For $T_{e,min}$ = 10eV the central RE current is ~10^{-2} of the total current density, and only 10^{-8} at r/a=0.75, not yet affecting σ.

But for Te,min=5eV, it reaches ratio 1.0 at plasma center! Minimum Te is possibly as low as 1 eV. Minimum Te dynamics needs careful study.

Future work:

.Couple the RE current back to NIMROD ==> should give a slower current quench.

.Include NIMROD stochastic mag field radial diffusion.

.Include time-dependent equilibrium into CQL3D.

Production rate of RE in time-dependent scenarios using BMC offers promise for integrated simulations

- An accurate computation of RE generation requires the incorporation of time dependent plasma conditions, e.g. T=T(t) and E=E(t).
- We have extended the BMC method to this type of time dependent scenarios
- The time evolution of the probability [**Fig.1**] and production rate [**Fig.2**] exhibit nontrivial dependence of the E field evolution [**Fig.3**]
- We have also extended the BMC method to incorporate spatial (diffusive) transport due stochastic magnetic fields.

Fig.1 **Probability of runaway at t=0.6**

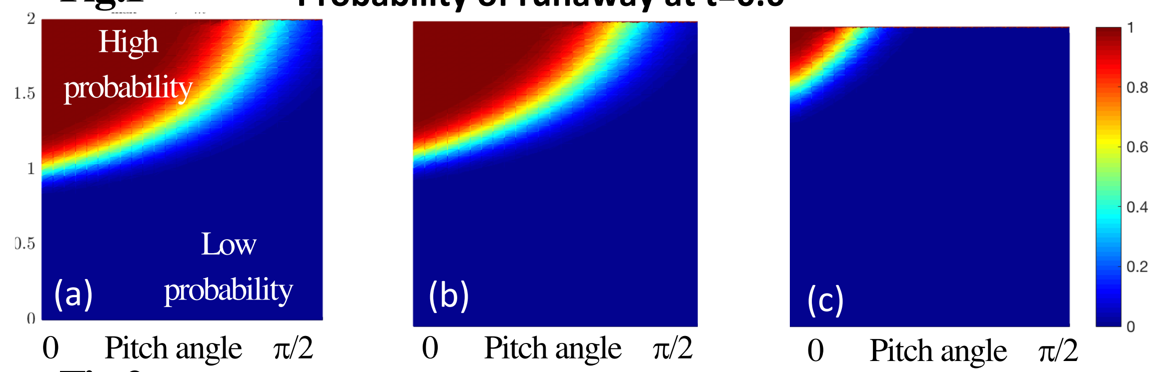


Fig.2

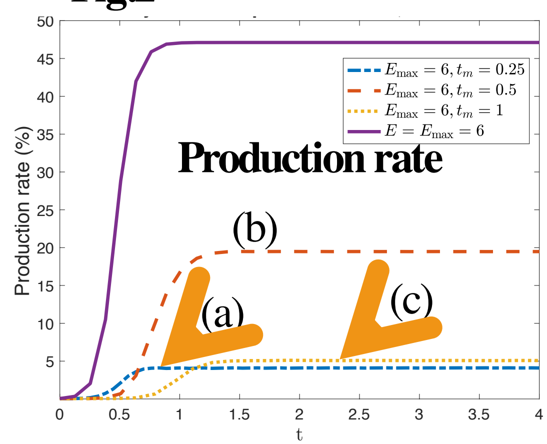
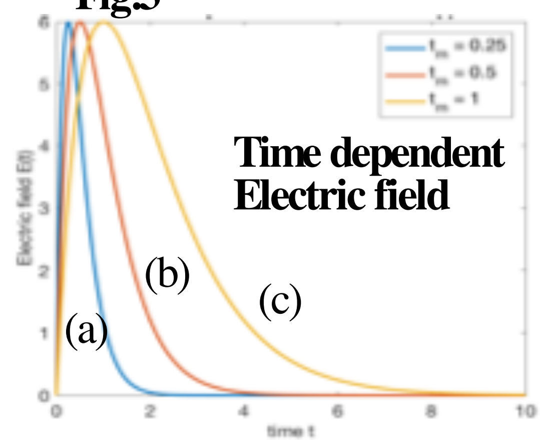


Fig.3



See also: E. Hirvijoki et al, **25**, 062507 (2018).

Zhang and del-Castillo-Negrete, Physics of Plasmas **24**, 092511 (2017).

Using M3D-C1 fields in KORC will offer further exploration of RE generation in diruption simulations

- KORC requires a fast, scalable method to interpolate background plasma conditions at particle positions.
  1. Interpolation is the current bottleneck when pushing particles.
  2. Interpolation needs to be thread safe and vectorizable for optimal scaling.
- Exploring two methods.
  - Interpolate M3D-C1 fields to a fixed rectangular grid.
    - Fast to interpolate using psplines at any point.
    - Reduced accuracy.
      - May not preserve $\nabla\cdot \mathbf{B} = 0$.
  - Direct integration of M3D-C1 interpolation routines into KORC.
    - Accurate
    - Slow for initial particle lookup or when particle cache misses.
- Benchmarking both methods for impact on particle pushing speed.

Collaboration between SCREAM and CTTS SciDAC

Coupling Backward Monte-Carlo to KORC

- The heaviest computation lies in the convolution of the runaway probability with the driving stochastic dynamics, i.e.,

$$\mathbb{E}\left[P_{\mathrm{RE}}(t_{n+1}, X_{n+1})\right] = \int_{\mathbb{R}^d} P_{\mathrm{RE}}\left(t_{n+1}, X_n + b\Delta t + \sigma \Delta W\right) d\rho(\Delta W),$$

which requires large number of

- Integration using Gauss-Hermite (GH) quadrature
- Interpolation at all the quadrature points, i.e., # mesh nodes → # GH quadrature abscissae (e.g., 27 abscissae per node)

Our Strategy:

- We implemented the GPU-enabled BMC method by coupling our code with the GPU sparse linear algebra library (cuSparse) in the following way:
  - Convert the Integration and Interpolation to large sparse-dense matrix multiplication
  - Accelerate such multiplication via a set of custom CUDA kernels

A central guiding objective within SCREAM is the development of a WDM module for runaway physics that will reliably predict mitigation strategies.

- This capability would require almost the full functionality of a whole device modeling (WDM) of a tokamak, and the physics studies currently being undertaken will naturally lead to a runaway physics module for WDM.
- Multiple approaches currently being investigated in SCREAM could be applicable to WDM functionality.
- Post disruption mitigation modeling, perhaps of most interest, would require 3D MHD and particle based modeling, perhaps with full wave calculations, essentially utilizing and extending beyond the most advanced computations within SCREAM.

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 (KORC+NIMROD and M3D-C1, CQL3D+NIMROD, +more)
  - 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 (0X-2V up to 3X-3V)
- Shattered pellet injection and ablation studies
  - Studying RE interaction with plume in 3D fields of MHD