Modeling and Simulation of Runaway Electron Dissipation by Impurity Injection Using KORC

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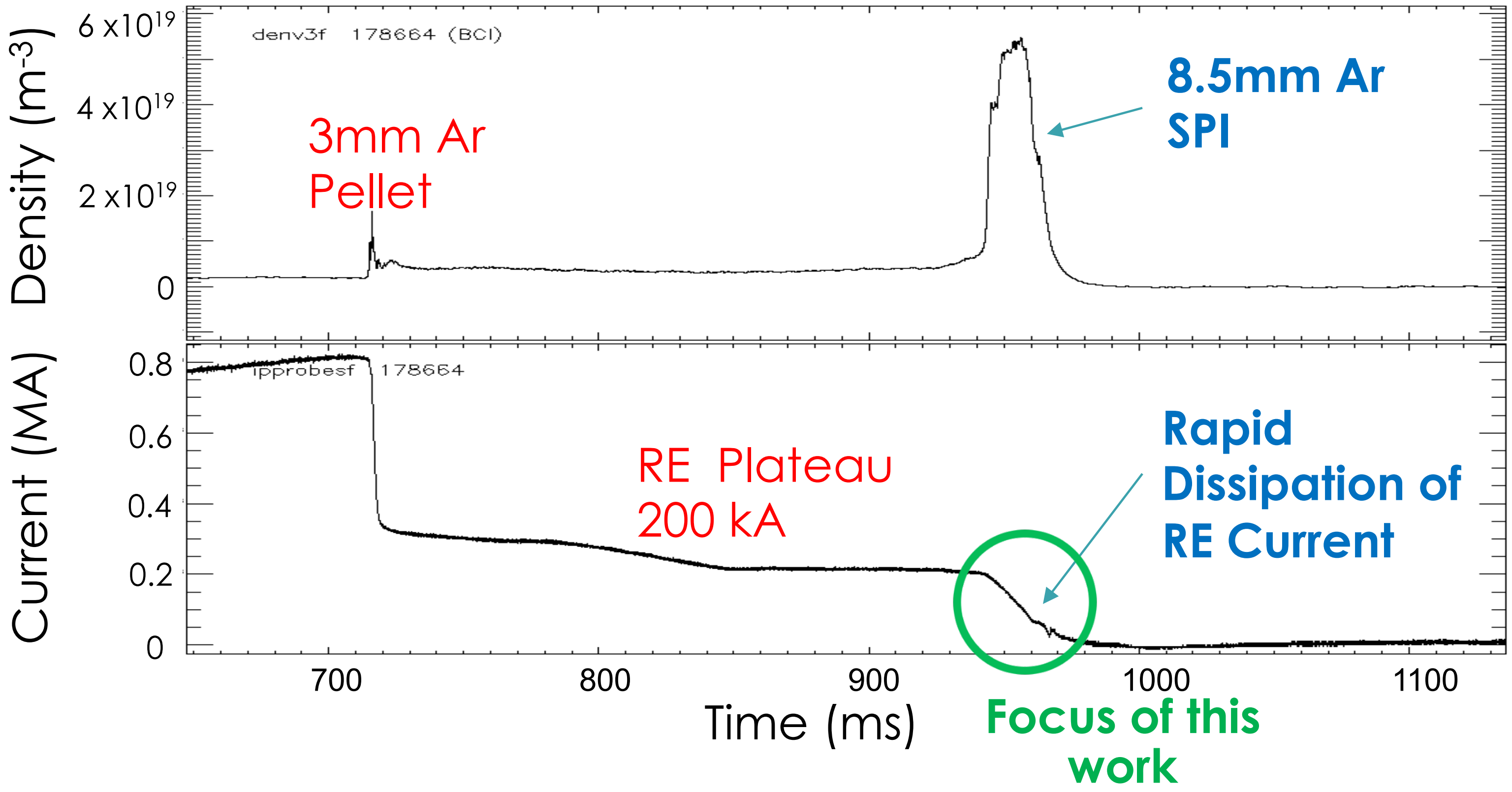
1: Oak Ridge National Laboratory 2: PPPL

Argon SPI into RE beam on DIII-D shot 178664 shows rapid dissipation of the RE current



- **Ar SPI has been used into a RE beam and shows the ability to collisionally dissipate the RE current on a 20-30 ms time scale**
  - Ar bound electrons and free electrons from ionization scatter REs
  - Approximately 15% assimilation rate of SPI

Main Results

- **Developed KORC for verification and validation of RE dissipation models**
  - RGC model that interpolates general magnetic field
  - Monte Carlo Coulomb collisions with bound electron models
  - Spatio-temporal partially-ionized and free electron density model and evolving electric field
- **Correct modeling of RE dissipation time scale requires:**
  - Bound electron model [*e.g.* Hesslow et al., *PRL* (2017)]
  - Spatio-temporal "penetrating ring" density model
  - Inductive electric field generated by slowing down collisions
    - Self-consistent model of E_{ind} presently being developed
- **Coupling of KORC and M3D-C1 is underway**
  - FO calculations use Fusion-IO M3D-C1 fields and can be used with a synchrotron emission synthetic diagnostic
  - RGC calculations presently developed for axisymmetric fields

Relativistic guiding center (RGC) equations are implemented in KORC

- **RGC system of equations evolved with Cash-Karp 5th order Runge-Kutta**

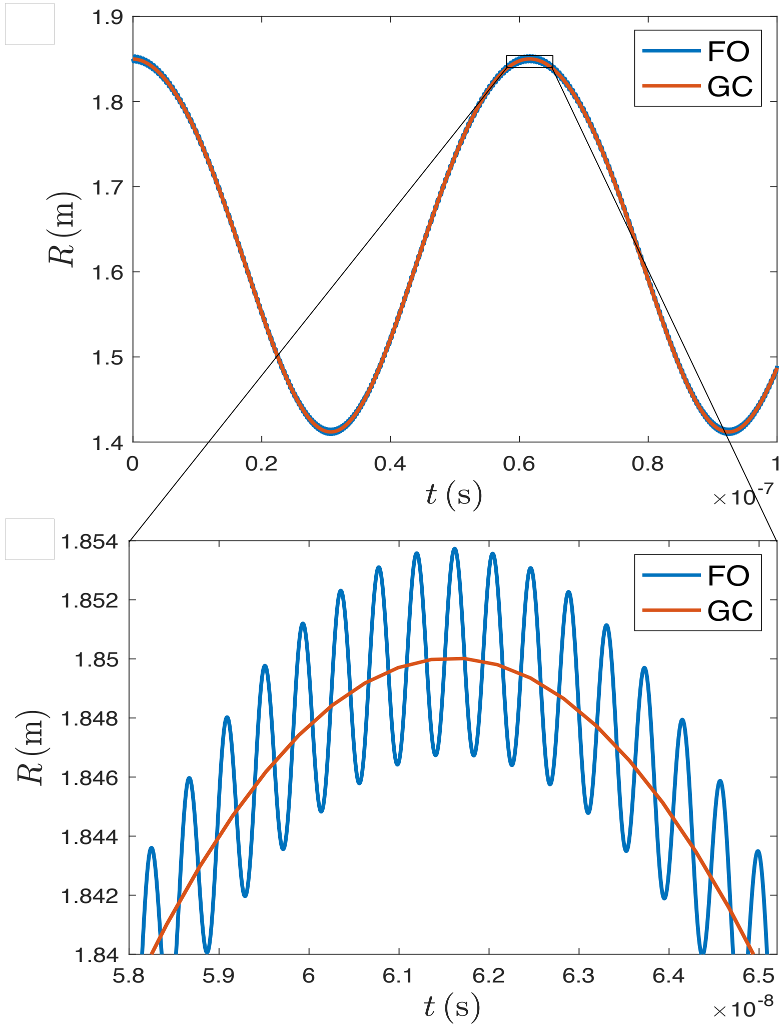
$$\frac{d\mathbf{X}}{dt} = \frac{1}{\mathbf{b}\cdot\mathbf{B}^*}\left(e\mathbf{E}\times\mathbf{b} + \frac{m_e\mu\mathbf{b}\times\boldsymbol{\nabla}B + p_\parallel\mathbf{B}^*}{m_e\gamma_{\mathrm{GC}}}\right),$$

$$\frac{dp_\parallel}{dt} = \frac{\mathbf{B}^*}{\mathbf{b}\cdot\mathbf{B}^*}\cdot\left(e\mathbf{E} - \frac{\mu\boldsymbol{\nabla}B}{\gamma_{\mathrm{gc}}}\right),\ \mu = \frac{|\mathbf{p}-p_\parallel\mathbf{b}|^2}{2m_eB} = \frac{p_\perp^2}{2m_eB},$$

$$\mathbf{B}^* = q\mathbf{B} + p_\parallel\boldsymbol{\nabla}\times\mathbf{b},\ \gamma_{\mathrm{gc}} = \sqrt{1+\left(\frac{p_\parallel}{m_ec}\right)^2 + \frac{2\mu B}{m_ec^2}}$$

  - Tao, Chan, and Brizard, *POP* (2007)
  - For static magnetic fields

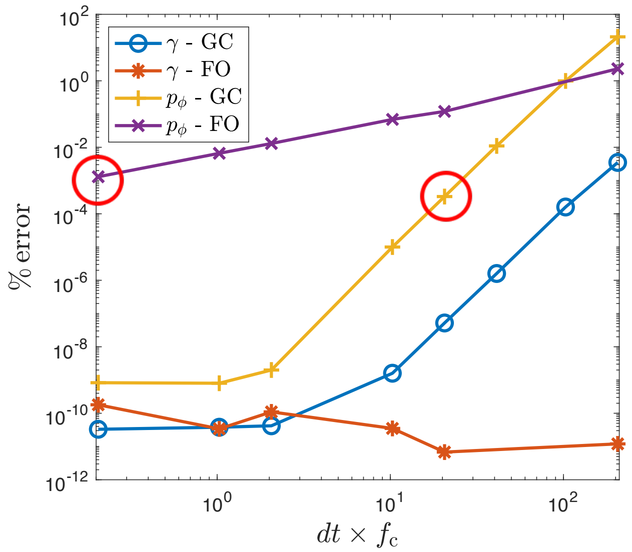
- **Evaluate analytic or general fields with PSPLINE interpolation routines**
  - Cubic spline interpolation for (possibly 3D) fields or potentials
  - Advances on KORC-GC which uses nested flux surfaces in Boozer coordinates



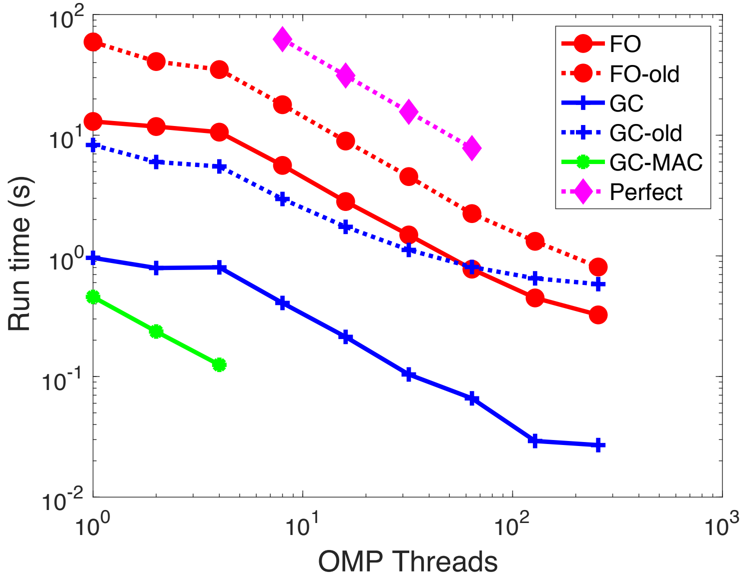
10 MeV passing particle

RGC equations of motion can be accurately integrated more rapidly than FO

- **Primary accuracy metrics are energy and toroidal canonical momentum for axisymmetry**
  - Single particle calculations evaluate axisymmetric analytical field for 1 ms
  - FO accuracy requirement is gyro-orbit
  - RGC accuracy requirement is particle drifts and parallel dynamics



- **HPC optimization to reduce OpenMP synchronization overhead and increase vectorization**
  - Strong scaling shown for field interpolation
  - Modest gains for FO
  - Over 20x faster for RGC



Monte Carlo Coulomb collision operator valid for thermal and relativistic particles

- **Stochastic differential equation (SDE) for Coulomb collision operator**

$$dp = \left[-C_F + \frac{1}{p^2}\frac{\partial}{\partial p}\left(p^2 C_A\right)\right] dt + \sqrt{2C_A} dW_p,$$

$$d\eta = \frac{C_B}{p^2}\cot\eta dt + \frac{\sqrt{2C_B}}{p} dW_\eta$$

  – dW is a Weiner process satisfying $< dW >= 0, \; < (dW)^2 >= dt$

- **Transport coefficients C_B, C_A, C_F are pitch-angle scattering, parallel diffusion, and slowing down**

$$C_B = \frac{p^2 \nu_D^{ei}}{2} + \frac{\nu_D^{ee}}{2} = \frac{\Gamma_{ei}}{2v} Z_{\text{eff}} + \frac{\Gamma_{ee}}{2v}\left[\text{erf}\left(\frac{v}{v_{th}}\right) - \psi\left(\frac{v}{v_{th}}\right) + \frac{1}{2}\left(\frac{v_{th} v}{c^2}\right)^2\right]$$

$$C_A = \frac{p^2 \nu_\parallel^{ee}}{2} = \frac{\Gamma_{ee}\psi\left(\frac{v}{v_{th}}\right)}{v}, \; C_F = \frac{p\nu_S^{ee}}{2} = \frac{\Gamma_{ee}\psi\left(\frac{v}{v_{th}}\right)}{T_e}$$

  – $\Gamma_{ee,ei} = \frac{n_e e^4 \ln\Lambda_{ee,ei}}{4\pi\epsilon_0^2}$, $\psi(x) = \frac{\text{erf}(x) - x\,\text{erf}'(x)}{2x^2}$

  – General forms from Papp et al., *NF* (2011)

  – Singularity in C_B as $v \to 0$

- **Coulomb logarithms for small angle collisions from Hesslow et al., *PRL* (2017) valid at relativistic limit**

$$\ln\Lambda_{ee} = \ln\Lambda_0 + \frac{1}{5}\left\{1 + \left[2(\gamma - 1)c^2/v_{th}^2\right]^{5/2}\right\},$$

$$\ln\Lambda_{ei} = \ln\Lambda_0 + \frac{1}{5}\left[1 + (2\gamma v/v_{th})^5\right],$$

$$\ln\Lambda_0 = 14.9 - \frac{1}{2} n_e (10^{20}\,\text{m}^{-3}) + \ln T\,(\text{keV})$$

- ***dt* subcycled at a different rate than orbit iterations**

Bound electron models for partially-ionized impurities greatly increase collisionality

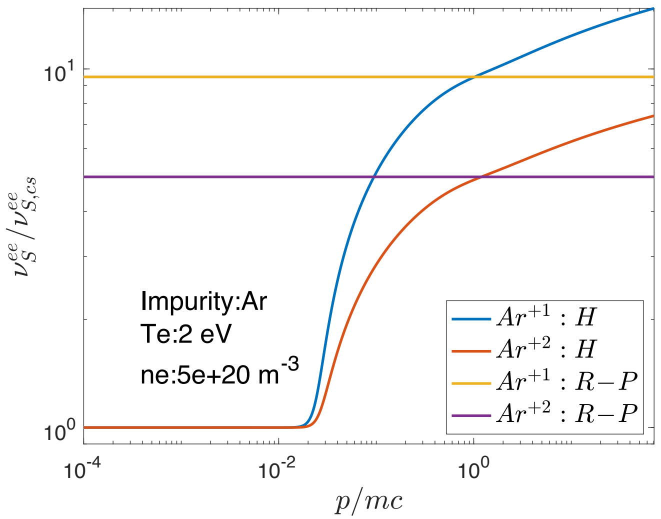
- **Bound electron effects incorporated into ν_S^{ee} and ν_D^{ei} in Hesslow et al., *PRL* (2017)**
- **Inelastic collisions slow down particles through ν_S^{ee}**
  - Hesslow (Bethe stopping-power):

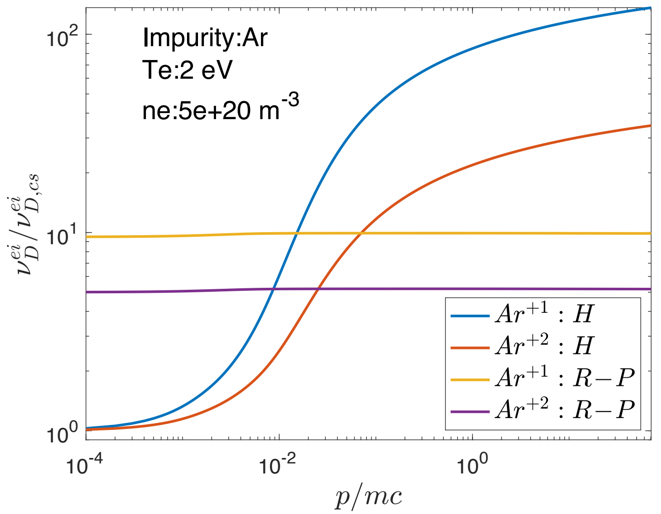
$$\nu_S^{ee} = \nu_{S,\mathrm{cs}}^{ee}\left\{1+\sum_j \frac{n_j}{n_e}\frac{Z_{0j}-Z_j}{\ln\Lambda_{ee}}\left[\frac{1}{5}\ln(1+h_j^5)-\beta^2\right]\right\},\ h_j = p\sqrt{\gamma-1}/I_j$$

    - I_j is mean excitation energy of impurity species j
    - Z_{0j} is fully ionized impurity charge
  - Rosenbluth & Putvinski (R-P): $\nu_S^{ee} = \nu_{S,\mathrm{cs}}^{ee}\left(1+\sum_j \frac{n_j}{n_e}\frac{Z_{j0}-Z_j}{2}\right)$
- **Elastic collisions with ions contribute to pitch angle scattering through ν_D^{ei}**
  - Hesslow (Born approximation):

$$\nu_D^{ei} = \nu_{D,\mathrm{cs}}^{ei}\left(1+\frac{1}{Z_{\mathrm{eff}}}\sum_j \frac{n_j}{n_e}\frac{g_j}{\ln\Lambda_{ei}}\right),\ g_j = \frac{2}{3}(Z_{0j}^2-Z_j^2)\ln(y_j^{3/2}+1)-\frac{2}{3}\frac{(Z_{0j}-Z_j)^2 y_j^{3/2}}{y_j^{3/2}+1},\ y_j = p\bar{a}_j$$

    - $\bar{a}_j$ is normalized effective ion scale length for impurity charge state
  - R-P: $\nu_D^{ei} = \nu_{D,\mathrm{cs}}^{ei}\left(1+\sum_j \frac{n_j}{n_e}\frac{Z_{j0}-Z_j}{2}\right)$



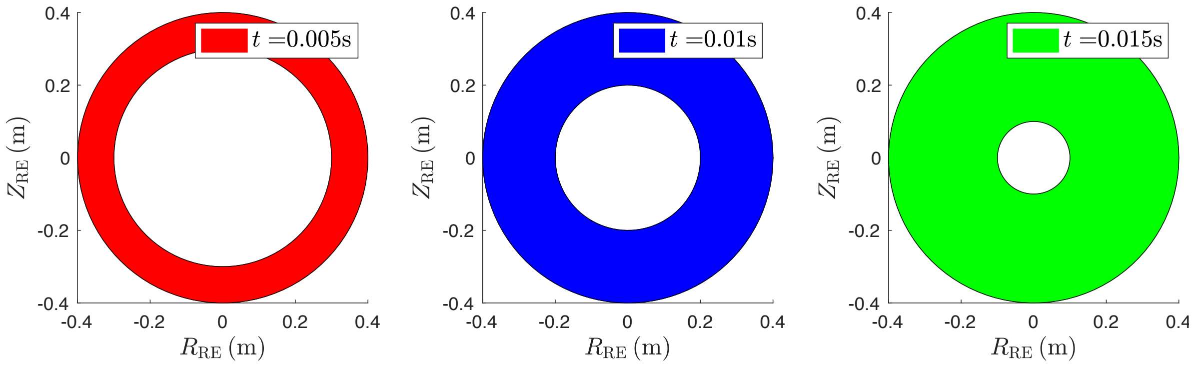


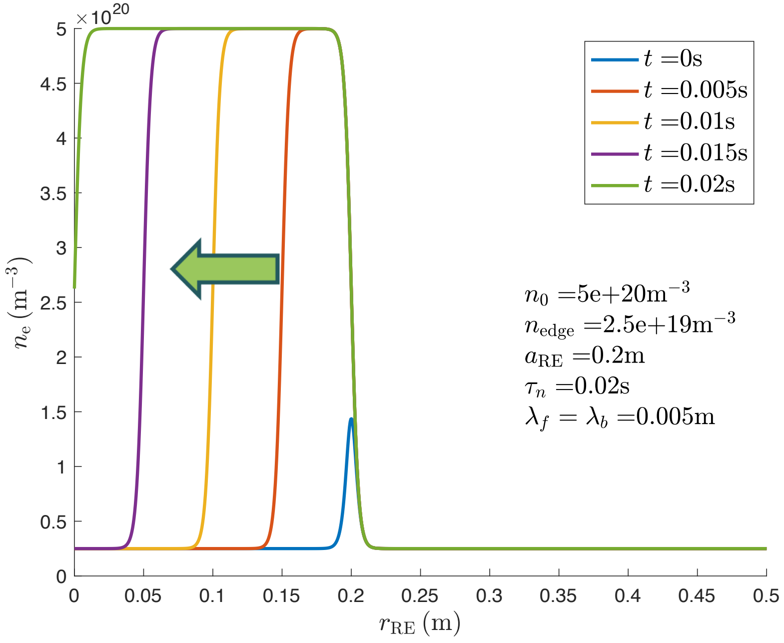
Spatio-temporally evolving electron density critical for modeling dissipation

- **Recent JET experiments indicate penetrating ring of high electron density as SPI plume interacts with RE beam**
- **Ad hoc model implemented into KORC to simulate penetrating ring n_e evolution**

$$n_e(r_{\mathrm{RE}},t) = \frac{n_0 - n_{\mathrm{edge}}}{4}\left[1+\tanh\left(\frac{r_{\mathrm{RE}} - a_{\mathrm{RE}}(1-t/\tau_n)}{\lambda_f}\right)\right] \times \left[1+\tanh\left(\frac{-(r_{\mathrm{RE}} - a_{\mathrm{RE}})}{\lambda_b}\right)\right] + n_{\mathrm{edge}}$$

  - Both free electron density and impurity density use same model
    - Assume %100 assimilation of SPI
  - Consistent with Ware pinch mechanism due to poloidal magnetic and inductive toroidal electric fields





Synchrotron radiation and toroidal electric field acceleration included through Cash-Karp method

- **Landau-Lifshitz representation of Lorentz-Abraham-Dirac radiation reaction force**

$$\mathbf{F}_{\mathrm{R}} = \frac{1}{\gamma\tau_R}\left[(\mathbf{p}\times\mathbf{b})\times\mathbf{b} - \frac{1}{(m_e c)^2}(\mathbf{p}\times\mathbf{b})^2\mathbf{p}\right], \quad \tau_R = 6\pi\epsilon_0(m_e c)^3/(e^4 B^2)$$

  - Written as equivalent SDE

$$\frac{dp_{\|}}{dt} = -\frac{p_{\|}(1-\cos^2\eta)}{\tau_R}\left(\gamma - \frac{1}{\gamma}\right),$$

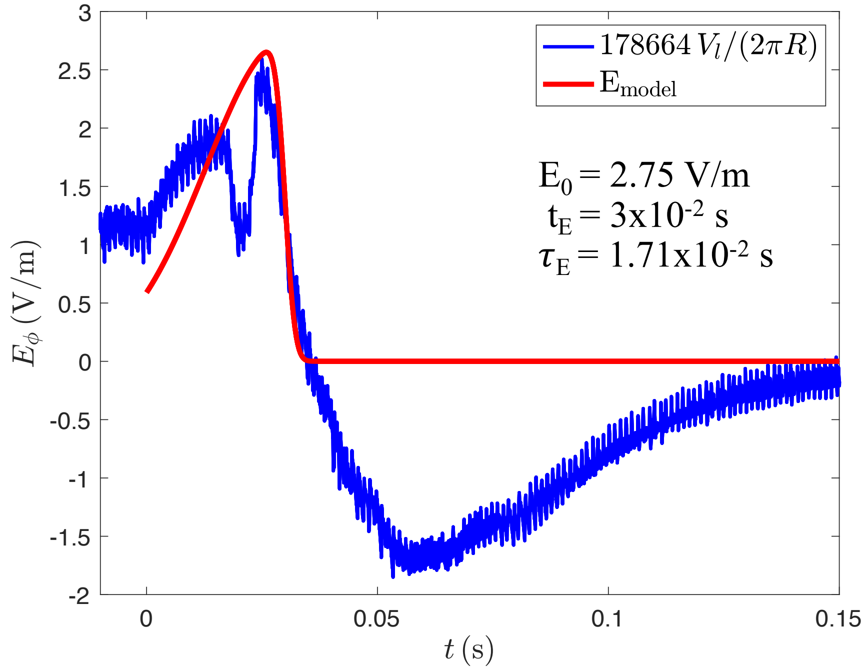
$$\frac{d\mu}{dt} = -\frac{2\mu}{\tau_R}\left[\gamma(1-\cos^2\eta) + \frac{\cos^2\eta}{\gamma}\right]$$

  - Small contribution for RE dissipation

- **Model toroidal electric field by fitting skewed Gaussian to 178664 loop voltage**

$$E_\phi(t) = E_0 \exp\left[-\frac{(t-t_E)^2}{2\tau_E^2}\right]\frac{1+\mathrm{erf}\left[-\frac{10(t-t_E)}{\sqrt{2}\tau_E}\right]}{2}$$

  - Self-consistent E_ϕ presently in development



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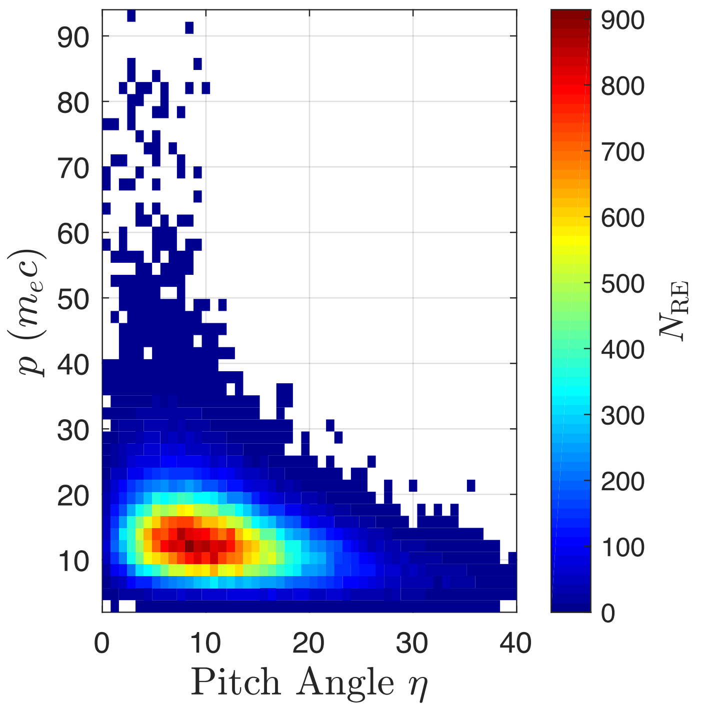
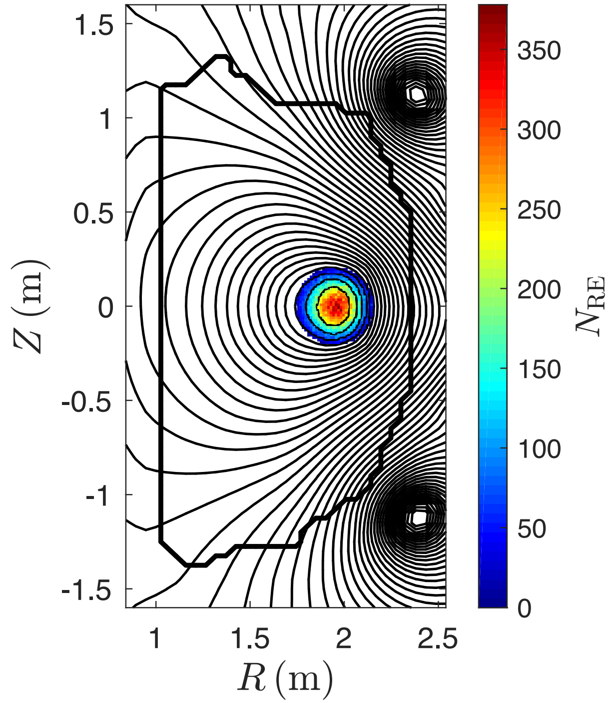
Initial conditions for simulations have RE beam centered at magnetic axis of DIII-D shot #178664

- **JFIT reconstruction at $t_0 = 942.17$ ms**
  - Interpolate ψ_p and all first and second order derivatives at each particle location to evaluate RHS of RGC equations
- **10^5 sampled REs**
  - Employ Metropolis-Hastings algorithm
  - Energy distribution inferred from DIII-D [Hollmann et al., *POP* (2015)]
- **n_e centrally peaked around 5×10^{19} m^{-3} falling to 2×10^{19} m^{-3} at edge**
- **T_e relatively flat at 1.5 eV**





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Bound electron collisions play significant role in RE dissipation

- **RE beam energy and current calculated as**

$$\mathcal{E}_{\mathrm{RE}}(t) = m_e c^2 \sum_i^{N_p} \gamma_i \mathcal{H}_{\mathrm{RE},i}(t),$$

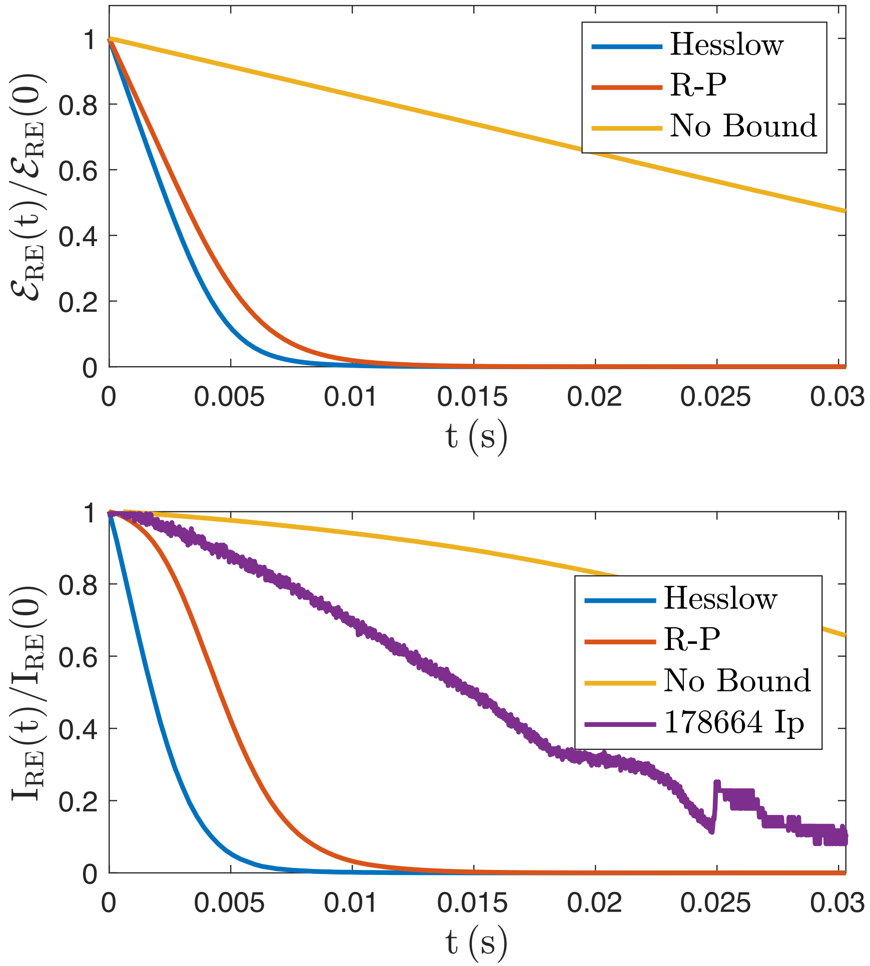
$$I_{\mathrm{RE}}(t) = e \sum_i^{N_p} v_{\parallel,i} \mathcal{H}_{\mathrm{RE},i}(t),$$

$$\mathcal{H}_{\mathrm{RE},i}(t) = \begin{cases} 1 & \text{if } p_i(t) > m_e c \\ 0 & \text{if } p_i(t) < m_e c. \end{cases}$$

  - REs hitting first wall also excluded

- **Simulations with flat, constant $n_e = 5\text{x}10^{20}\ \mathrm{m}^{-3}$**

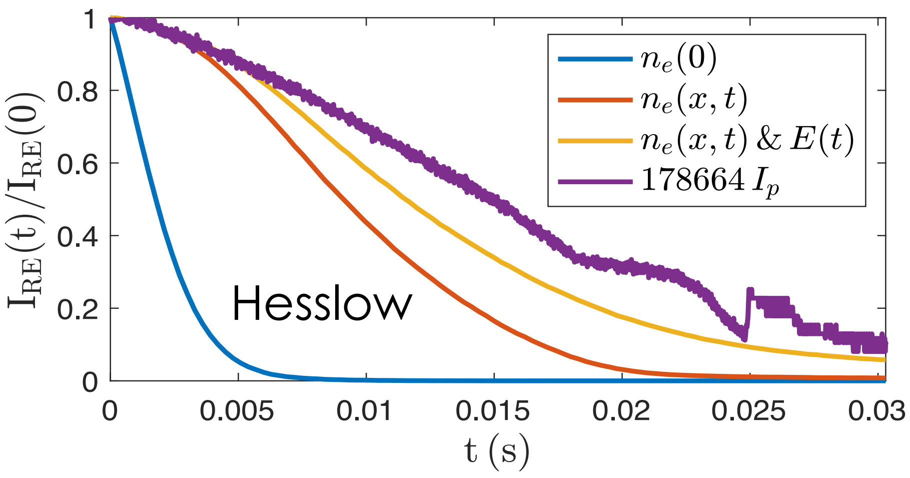
- **Dissipation time scale requires bound electron physics**

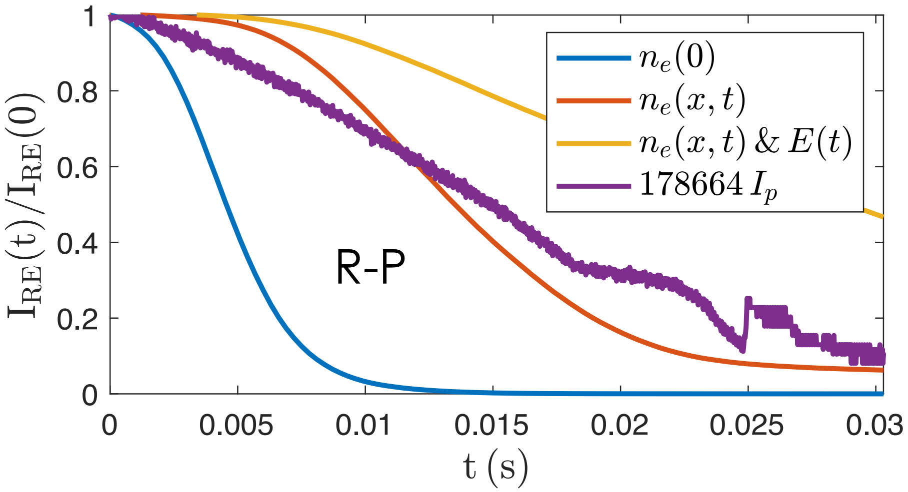


Spatio-temporal density profile and electric field evolution needed for recovering accurate RE dissipation

- **Regardless of bound electron model, spatio-temporal density profile and electric field evolution are dominant drivers of RE current dissipation**

- **KORC framework can be easily adapted to more complete bound electron models as they become available**

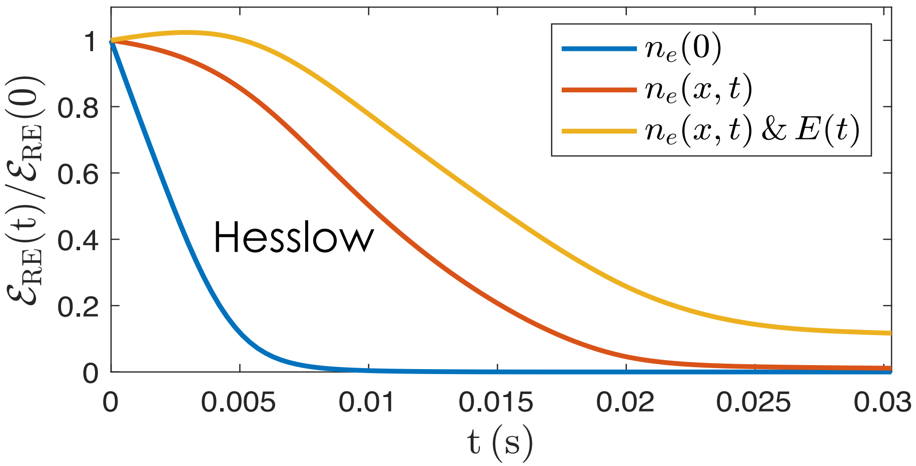


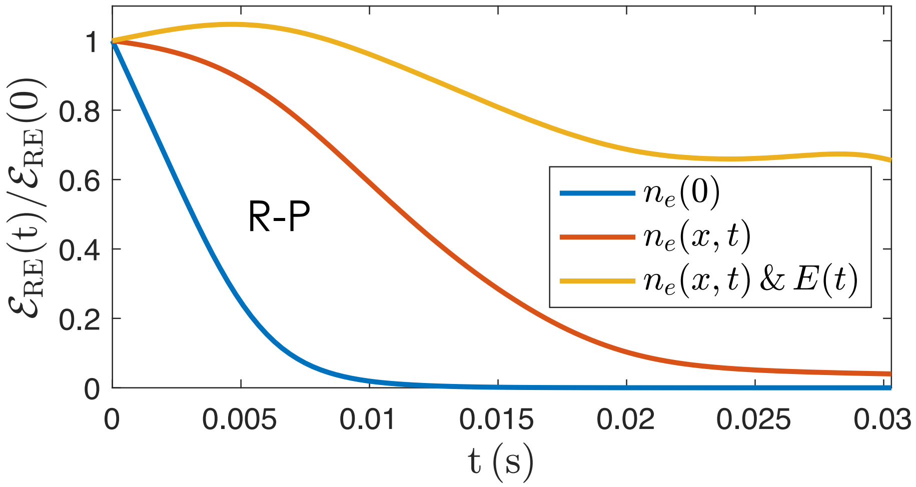


RE beam energy dissipation is qualitatively similar to current dissipation

- **Time evolution of RE beam current can be measured experimentally, but critical to know energy evolution**

- **Energy takes longer to dissipate because it is insensitive to pitch angle dispersion**
  - Electric field initially accelerates REs





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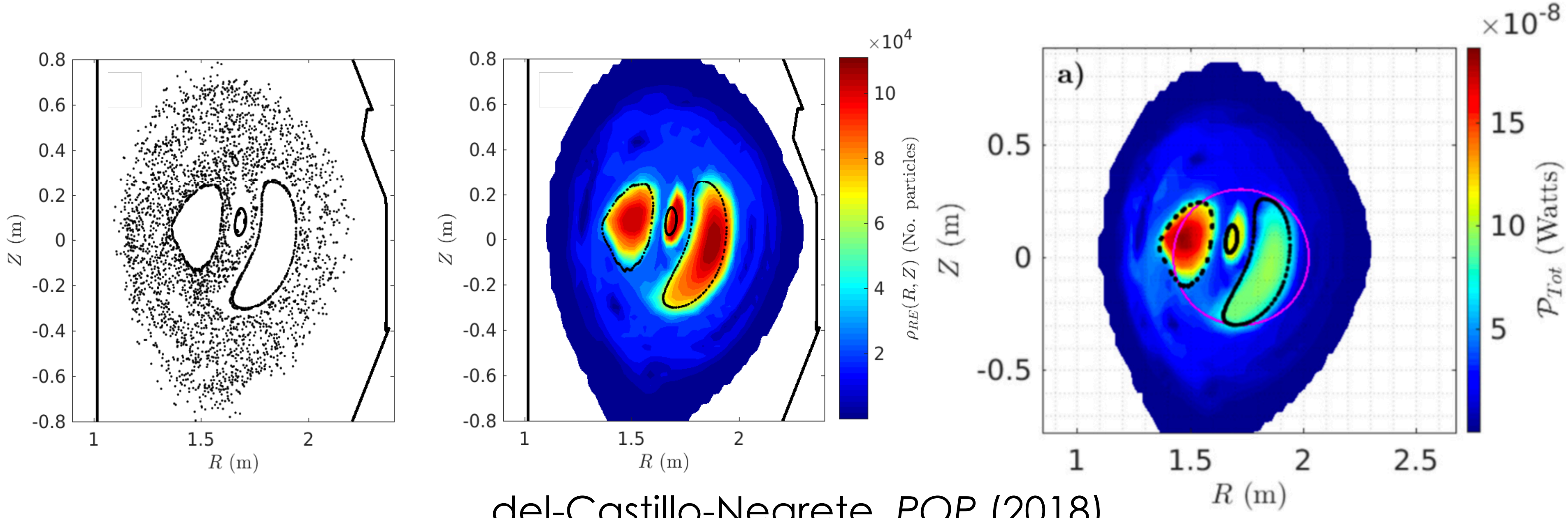
Previous SCREAM-CTTS activities include trace-particle coupling between KORC and NIMROD

- **FO calculations initialized from NIMROD simulations of DIII-D rapid shutdown scenario with MGI/SPI [Izzo et al., NF (2011)]**
- **REs confined in islands, lost from stochastic region**
- **Synchrotron emission (SE) synthetic diagnostic shows increased signal on HFS due to pitch angle dependence**



del-Castillo-Negrete, *POP* (2018)

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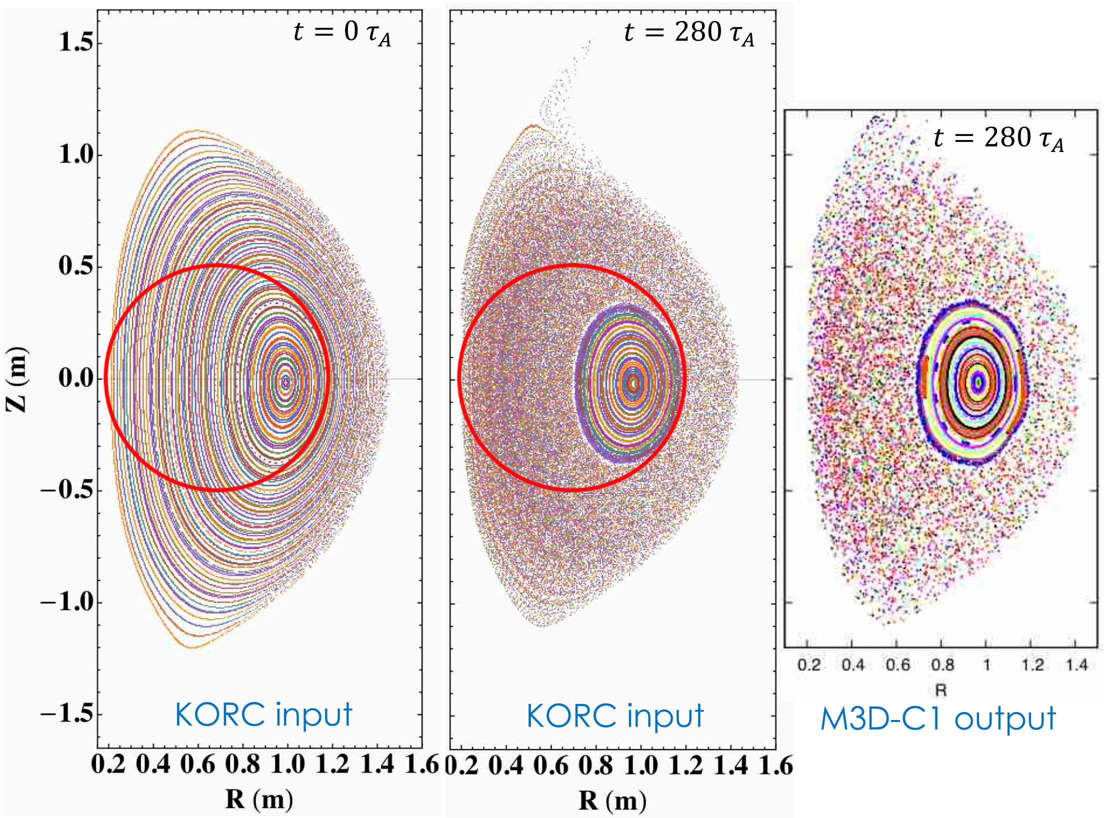
Efforts to couple KORC and M3D-C1 presently focus on two development pathways

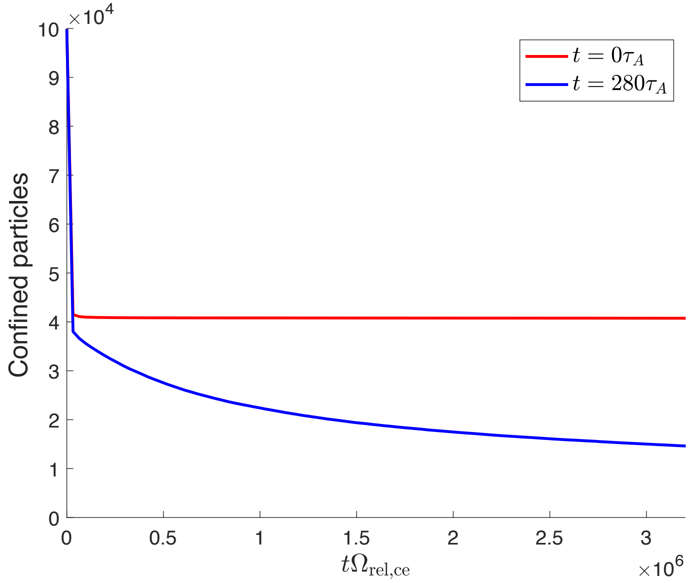
- **KORC FO calculations require field information**
  - Mark Cianciosa has been iterating with Nate Ferraro to adapt the Fusion-IO API for KORC field interpolation
  - Presently, precomputing fields with Fusion-IO then interpolating with PSPLINES yields best performance
  - FO calculation outputs can be used as inputs for synchrotron emission synthetic diagnostic
- **KORC RGC calculations require field and gradient information**
  - Accuracy of orbits is highly sensitive to input field fidelity, and even more so when field gradients are needed
  - 2D and 3D calculations have been performed
    - Use the M3D-C1 solution field ψ for 2D, derived field $\vec{B}$ for 3D
    - PSPLINES are used to calculate first and second order derivatives

KORC FO calculations have been performed with closed and stochastic 3D fields from M3D-C1

- **Poincare plots of M3D-C1 fields and KORC input fields show qualitative agreement**



- **Initialize uniformly distributed, monoenergetic (25MeV), monopitch (10°) RE beam (within red circle)**
- **Prompt loss of confinement due to drift orbit effects, gradual loss due to stochastic fields**



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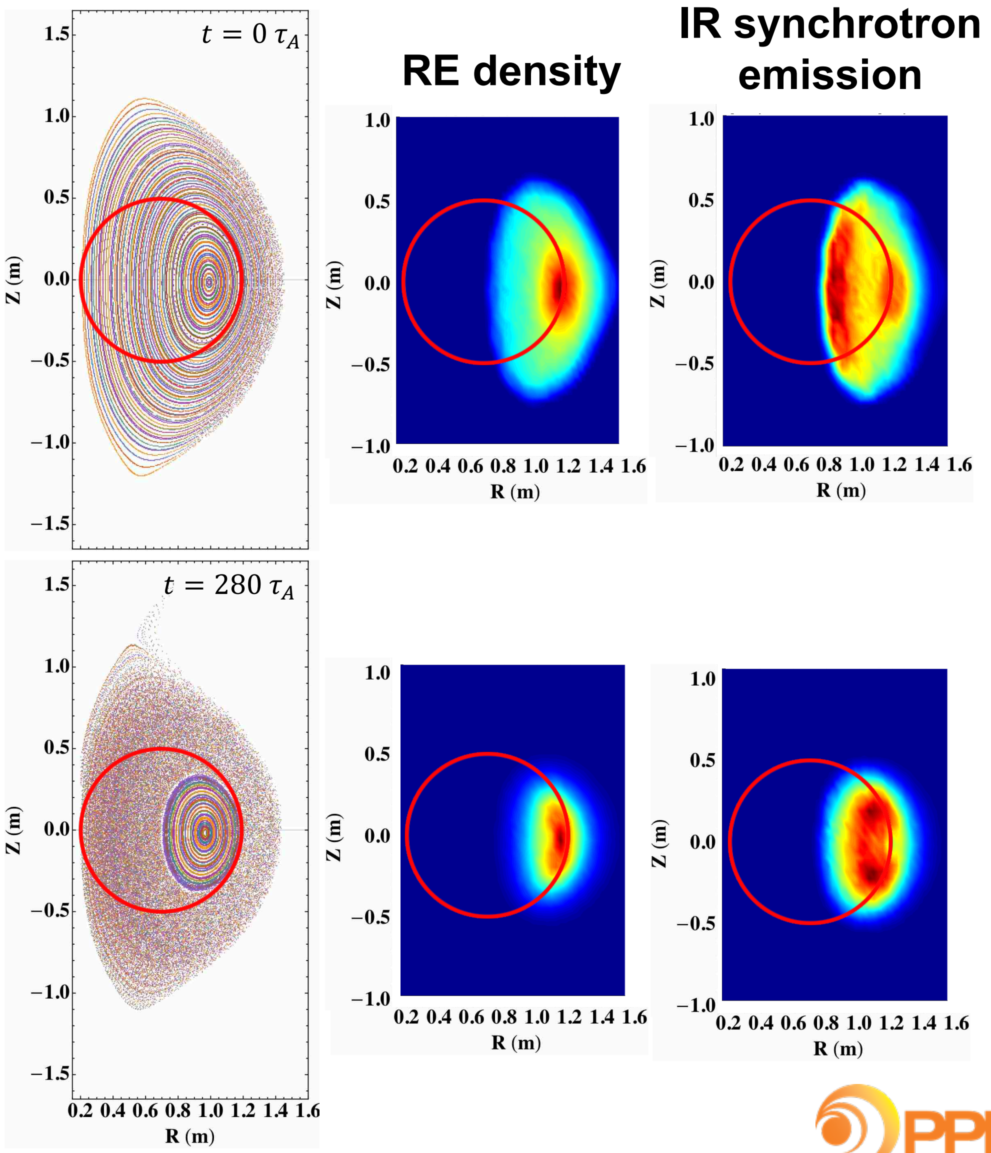
FO calculations can be used as inputs to SE synthetic diagnostic

- **After prompt loss phase, average over time to obtain good statistics for SE synthetic diagnostic**
- **RE density and infrared (IR) SE shown in poloidal plane**
  - Drift orbit effects cause maximum density to shift to LFS of magnetic axis
  - Pitch angle dependence of SE causes signal to be larger on HFS



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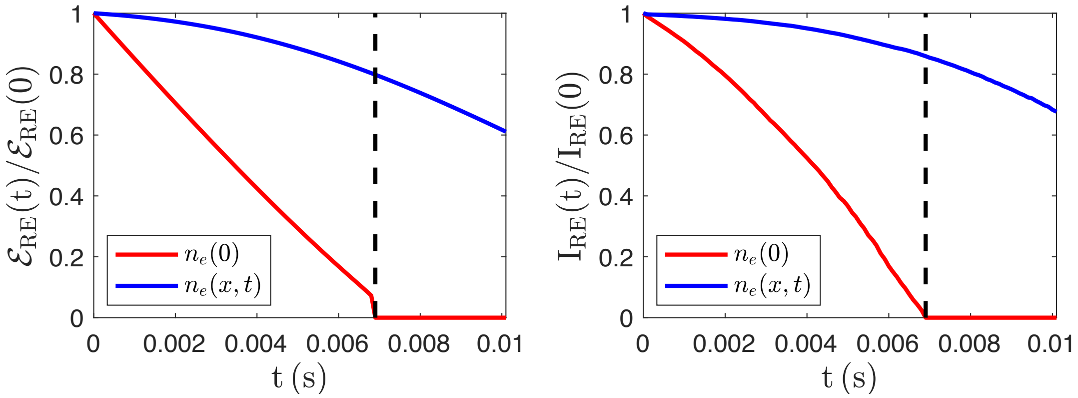
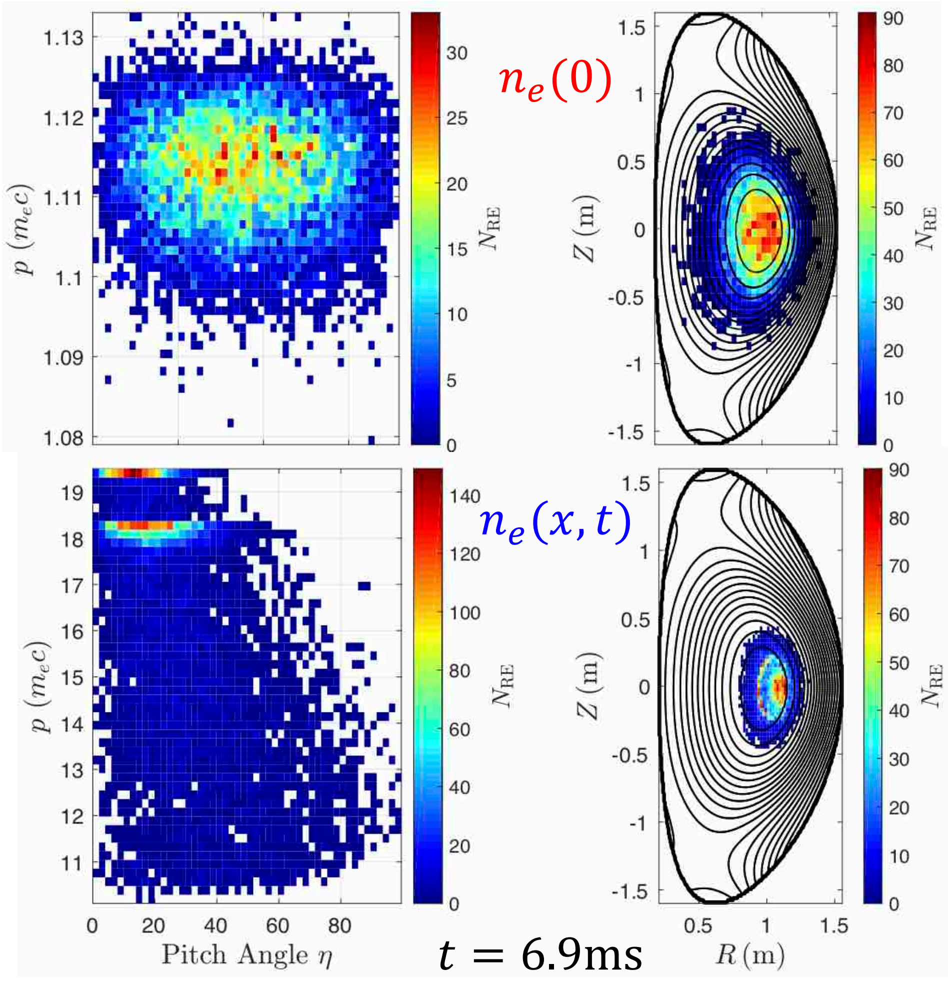
RE dissipation calculations show how spatio-temporal density profile affects energy and spatial distribution

- **Initialize 2D Gaussian distributed at magnetic axis, monoenergetic (10 MeV), monopitch ($10°$) RE beam**
- **Using Hesslow bound electron model, calculations with flat and spatio-temporal density profile, RE current evolves qualitatively similar to DIII-D case**
- **Spatio-temporal density profile causes multiple energy beams to form**





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General framework developed in KORC can be applied to general simulation of REs

- **Direct application**
  - Optimization of SPI deposition for RE mitigation
  - Interaction of REs with high frequency waves
  - Modeling seed runaway generation
- **Development needed**
  - Modeling knock-on (avalanche) RE growth
  - Fluid-kinetic coupling to MHD simulation of disruptions
- **Conceptual**
  - Energetic particle transport

KORC can be used for verification and validation of RE physics models

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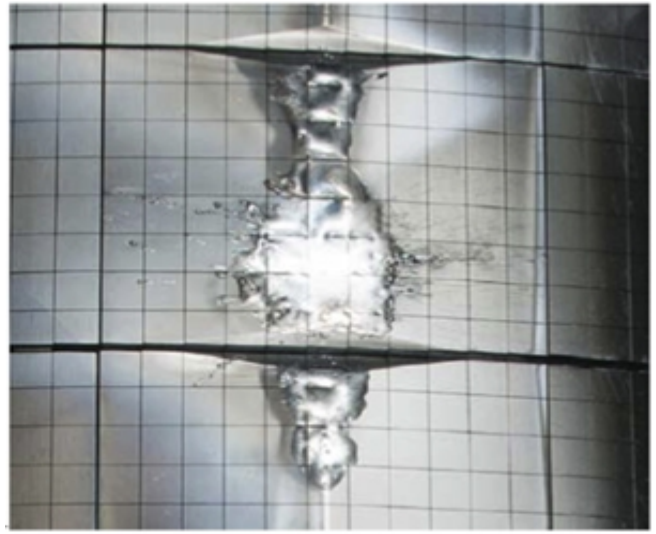
Extra Slides

Motivation

- **Tokamak disruptions can accelerate significant runaway electron (RE) population**
  - Large inductive electric field and impurity content
  - Increased stored energy and plasma current in future devices

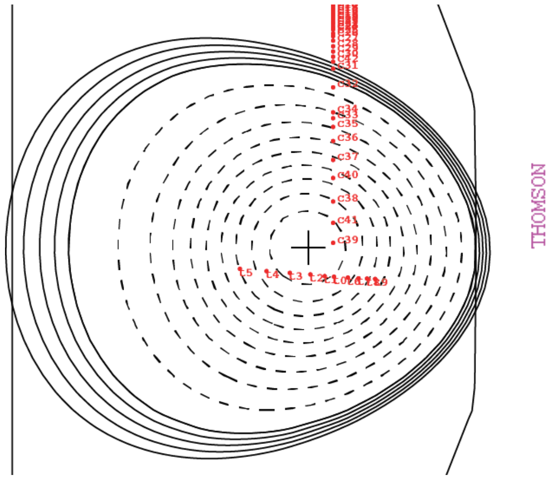


Damage to JET-ILW from REs
Matthews et al., *Phys. Scr.* (2016)

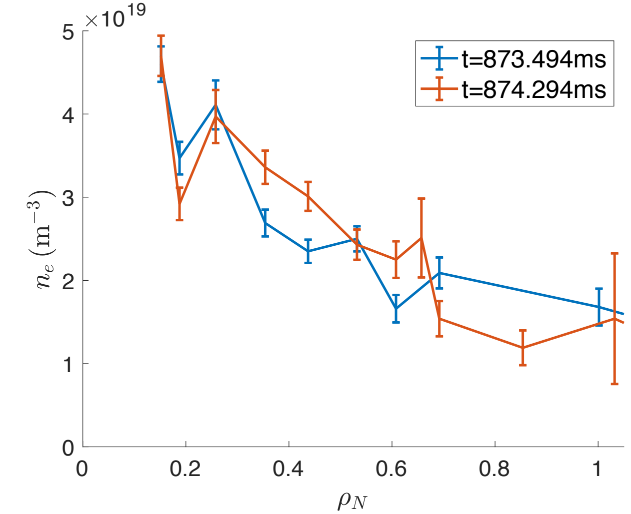
- **Shattered pellet injection is leading candidate for mitigation of REs**
  - Experiments ongoing at DIII-D, JET, and KSTAR to assess feasibility using pre-planned, forced disruptions
  - KORC can be used for verification and validation of RE dissipation models, and predictive modeling of SPI deployment
- **KORC developed for full orbits (FO), which are prohibitively computationally expensive for collisional processes**
  - While KORC-GC uses guiding center orbits, magnetic field must be concentric flux surfaces in Boozer coordinates

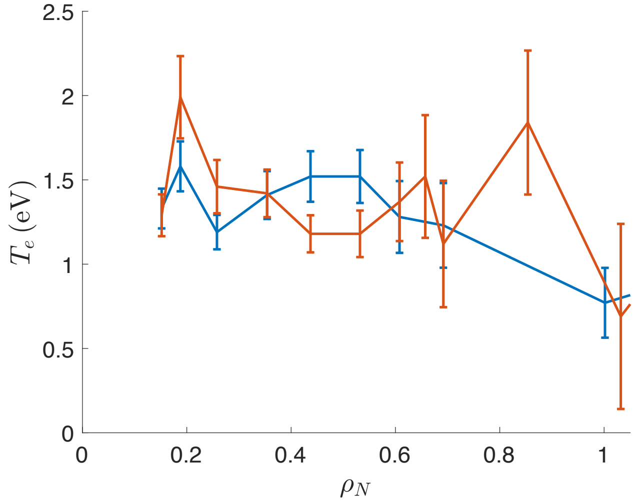
Thomson scattering data from RE plateau sets baseline for collision physics in DIII-D

- **Thomson scattering yields profile data of n_e and T_e during RE plateau**



- **n_e centrally peaked around 5×10^{19} m^{-3} falling to 2×10^{19} m^{-3} at edge**
  - Collisionality scales nearly linearly with n_e
  - KORC initialized with fit to profile
- **T_e relatively flat at 1.5 eV**
  - Collisionality scales weakly with T_e for $v >> v_{th}$





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Initial RE distribution sampled according to experimentally-inferred energy distribution

- **Desired distribution function**

$$f(r_{\rm RE},\mathcal{E},\eta) = f_{\mathbf{r}}(r_{\rm RE}) f_\eta(r_{\rm RE},\mathcal{E},\eta) f_{\mathcal{E}}(\mathcal{E}),$$

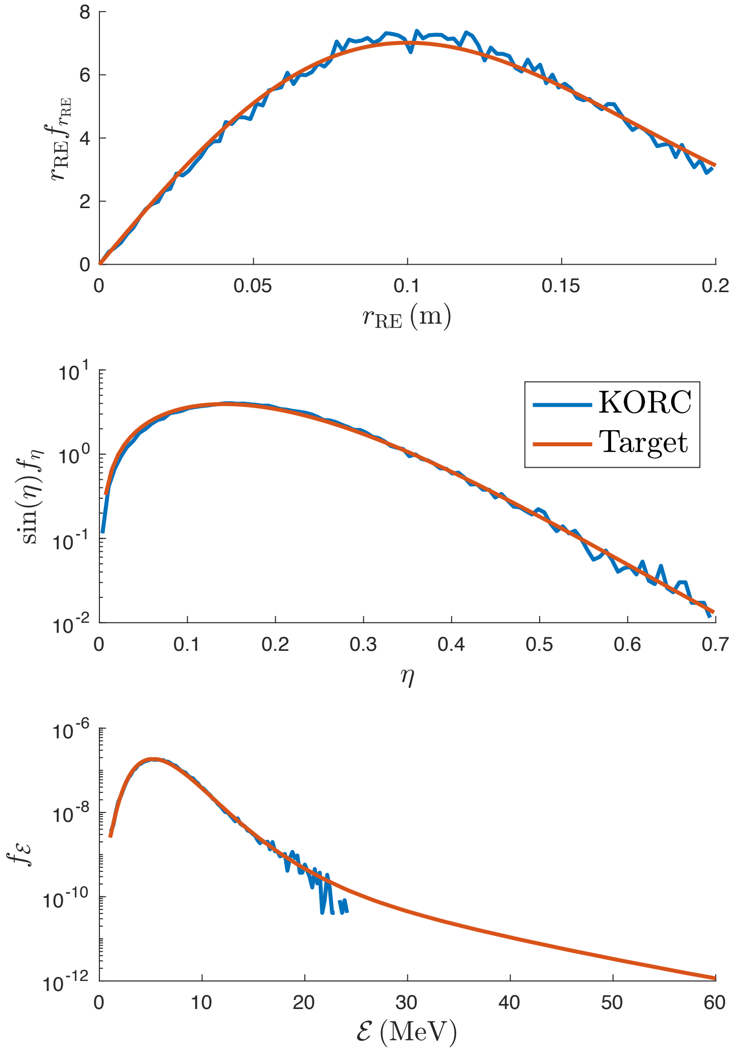
$$f_{\mathbf{r}}(r_{\rm RE}) = \mathcal{N}\exp\left(-\frac{r_{\rm RE}^2}{2\sigma_r^2}\right),$$

$$f_\eta(r_{\rm RE},\mathcal{E},\eta) = \frac{A}{2\sinh A}\exp(A\cos\eta),\ \ A(r_{\rm RE},\mathcal{E}) = \frac{2E(r_{\rm RE})}{Z_{\rm eff}(r_{\rm RE})}\frac{\gamma^2-1}{\gamma},$$

$$f_{\mathcal{E}}(\mathcal{E}) = f_H(\mathcal{E})$$

  - f_η is standard pitch angle distribution [*e.g.* Aleynikov and Breizman, *PRL* (2015)]
  - f_H from Hollmann et al., *POP* (2015)

- **Employ Metropolis-Hastings algorithm to initialize general, multidimensional, RE distribution**
  - Monte Carlo, Markov chain algorithm for sample selection
  - Evaluate distribution function multiplied by phase-space Jacobian



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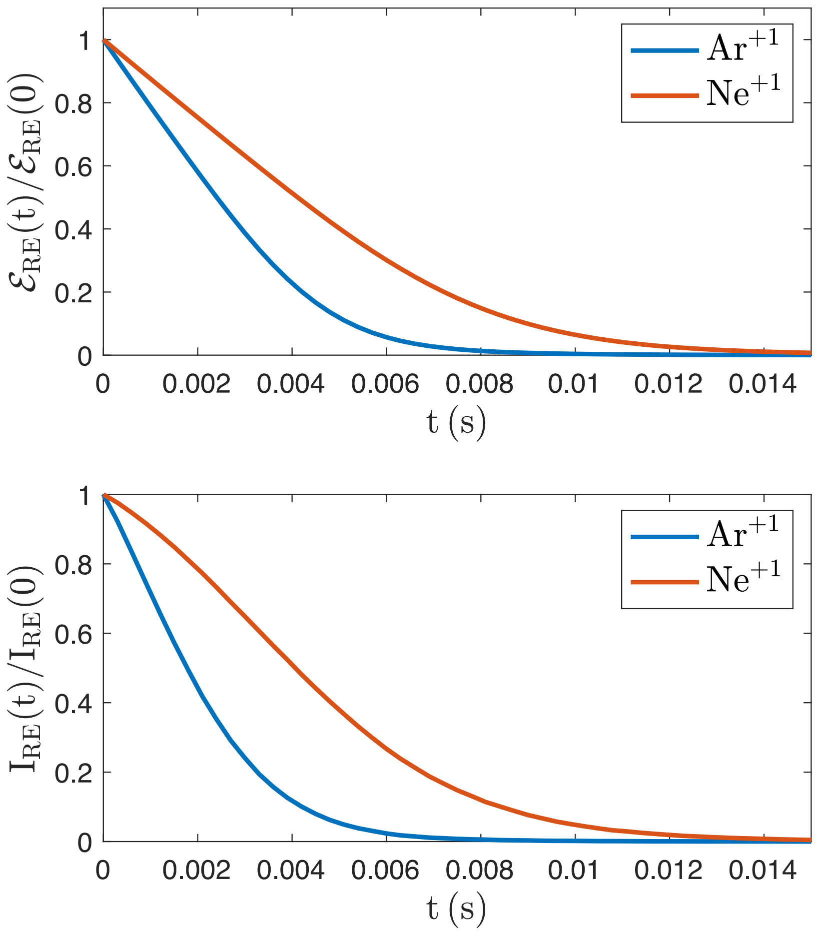
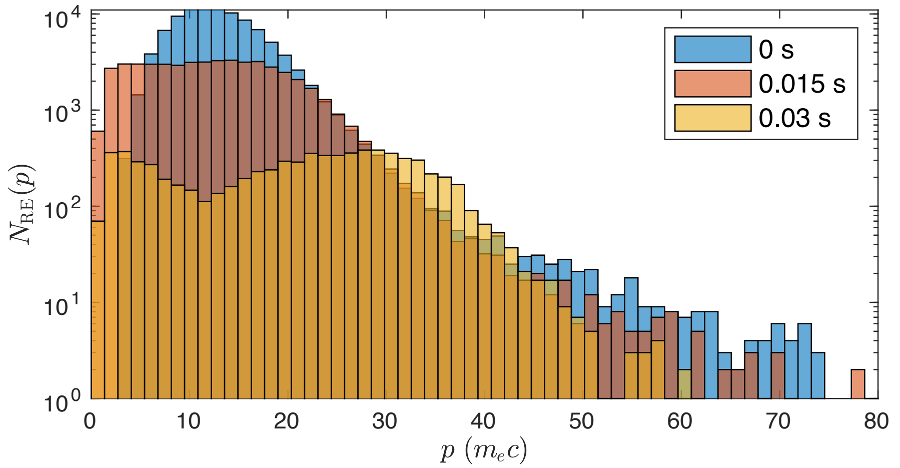
Increased number of bound electrons in injected impurity species enhances dissipation

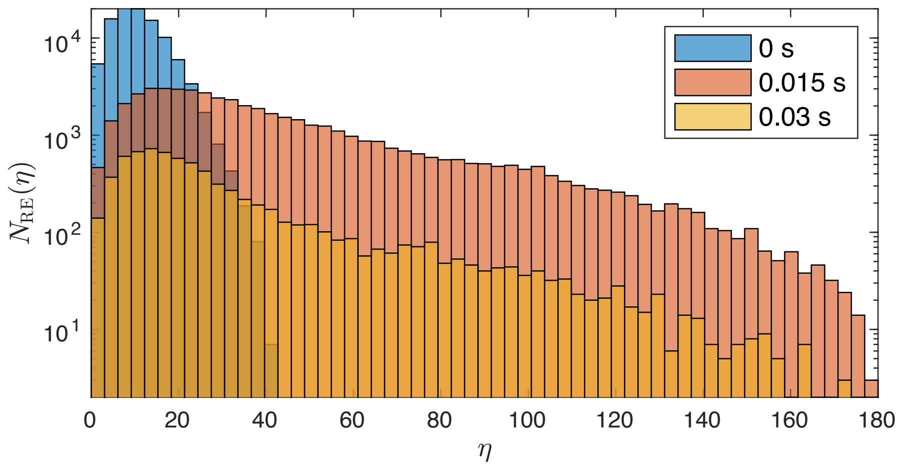
- **Ar causes RE beam to decay approximately twice as fast as Ne**
  - Consistent with there being nearly twice as many bound electrons
- **If damping REs is the only consideration in selecting an impurity for SPI/MGI, higher atomic number is better**
  - Creation, injection, ablation, ionization, and radiation are also important considerations



Energy dependence on collisionality and electric field govern RE energy distribution evolution

- **Histograms shown for Hesslow bound electron model with spatio-temporal density and electric field evolution**
- **As REs energy and pitch are dissipated, particles thermalize**
  - Removed from calculation when $p < m_e c$
- **Evolving electric field has a larger affect on high energy particles which are less collisional**





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REs are distributed along flux surfaces and are sensitive to spatio-temporal density profile

- **Histograms shown for Hesslow bound electron model with spatio-temporal density and electric field evolution**
- **On short time scale, spatial redistribution along flux surfaces**
- **Spatio-temporal density profile ring has maximum radius 0.2 m from initial center of RE beam**