Modeling of off-axis runaway electron generation in MST experiments

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Theory and Modeling Group
Fusion Energy Division
ORNL

CTTS Meeting
During APS-DPP
Spokane, Washington
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Work done in collaboration with:

ORNL

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PPPL

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- J. S. Sarff
- C. B. Forest

RE generation problem

- For a given plasma state (temperature drop, electric field evolution, magnetic field stochasticity, etc...), how many electrons become runaways before the second generation (avalanche) kicks in?
- Not knowing this is one of the weakest links in the assessment of the potential dangers of runaways in ITER and beyond
- The exponential growth predicted/assumed in the avalanche second generation process depends critical on the seed density
- The seed production depends on not well understood process including the nontrivial spatiotemporal evolution of the magnetic field stochasticity and the plasma cooling history
- This problem is one of the main deliverables of the DOE Theory Performance Targets for the SCREAM SciDAC project

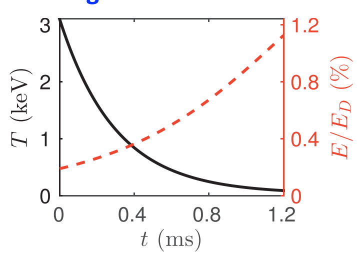
STANDARD APPROACH FOR THE COMPUTATION OF SEED RE DENSITY

- Solve the FP equation for a Maxwellian i.c. to get $f(\mathbf{r}, \mathbf{p}, t)$
- Prescribe the "runaway region", Ω_{RE}, based on a model and/or physical intuition
- Integrate $f(\mathbf{r}, \mathbf{p}, t)$ over the runaway region

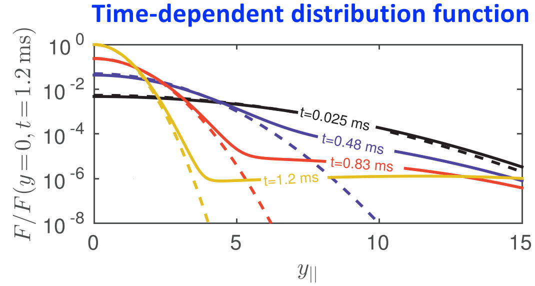
$$n_{RE}(t) = \int_{\Omega_{RE}} f(\mathbf{r}, \mathbf{p}, t)\, d\Omega$$

Example (among several others in the literature):

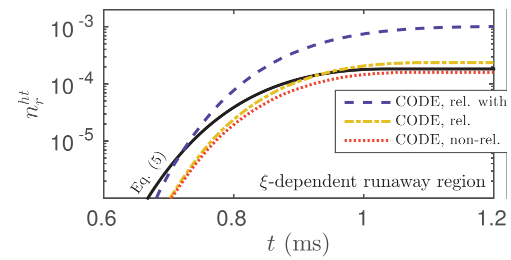
Cooling model and E field



Time-dependent distribution function



Seed runaway electron density

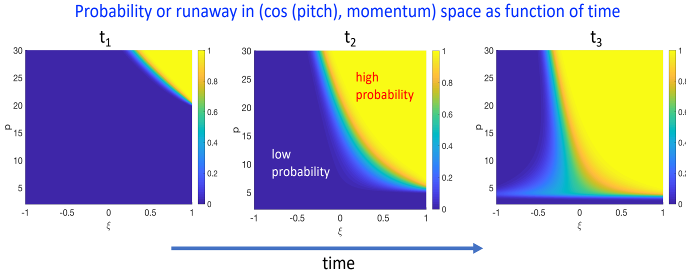


A. Stahl, et al., Nucl. Fusion **56** (2016) 112009

RE generation problem: Probabilistic approach

Compute the probability, P_{RE}, that an electron located at $(\mathbf{r}, \mathbf{p})$ will runaway at or before time t and integrate over the whole space

Probability or runaway in (cos (pitch), momentum) space as function of time

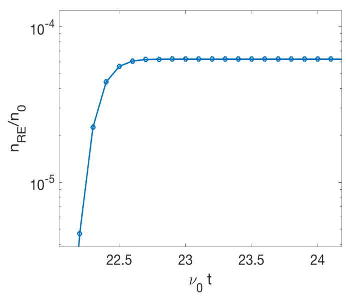


RE seed density

$$n_{RE}(t) = \int P_{RE}(\mathbf{r}, \mathbf{p}, t)\, f_0(\mathbf{r}, \mathbf{p})\, d\Omega$$

Probability of runaway

Initial condition e.g., Maxwellian



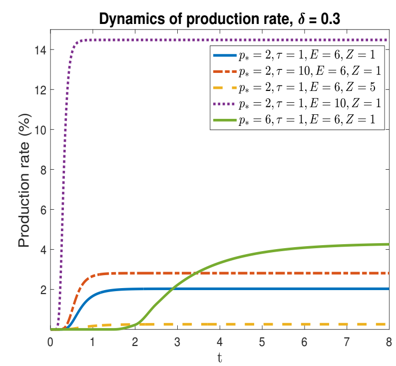
RE seed production can be directly evaluated for **any** initial condition, allowing the **fast evaluation of different i.c. scenarios**

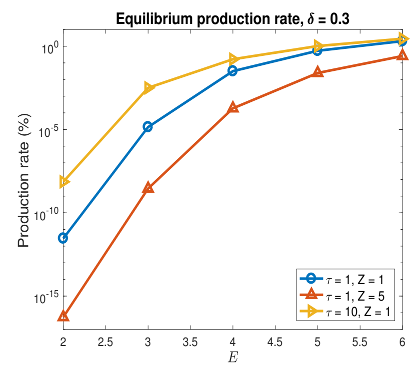
PRODUCTION RATE

$$\gamma = \frac{N_{\rm RE}(t)}{N} = \int_0^\infty dp \int_{-1}^{1} d\xi\, f(p,\xi) P_{\rm RE}(t,p,\xi)\,.$$

For a Maxwellian distribution

$$\gamma(t) = \frac{2}{\sqrt{\pi}\delta^3} \int_0^{p_*} dp\, e^{-(p/\delta)^2} p^2 \int_{-1}^{1} d\xi\, P_{\rm RE}(t,p,\xi) + \gamma_\infty\,,$$





Radiation reaction force $\sim 1/\tau$, collisions $\sim Z$, acceleration $\sim E$.

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ADVANTAGES OF THE PROBABILISTIC APPROACH: P_{RE} IS INDEPENDENT OF THE INITIAL CONDITION

- An advantage of the probabilistic approach is that P_{RE} is a kind of **Green's function** for the RE seed density computation
- That is, once P_{RE} is computed, the RE seed production can be directly evaluated for **any** initial condition, f_0, by simply doing the integral

$$n_{RE}(t) = \int P_{RE}(\mathbf{r}, \mathbf{p}, t)\, f_0(\mathbf{r}, \mathbf{p})\, d\Omega$$

- This allows the **fast evaluation of different i.c. scenarios**
- On the other hand, in the standard approach, for each initial condition, $f_0(\mathbf{r}, \mathbf{p})$, we have to solve the whole time-dependent Fokker-Planck initial value problem to get $f(\mathbf{r}, \mathbf{p}, t)$

$$n_{RE}(t) = \int_{\Omega_{RE}} f(\mathbf{r}, \mathbf{p}, t)\, d\Omega$$

- In the probabilistic approach, the runaway region $\Omega_{RE}(\mathbf{r}, \mathbf{p}, t)$ corresponds to the region where $P_{RE}(\mathbf{r}, \mathbf{p}, t) \sim 1$
- In 3D (p, ζ, r), the boundary of $\Omega_{RE}(\mathbf{r}, \mathbf{p}, t)$ is not sharp and its time-dependent shape can be highly nontrivial.
- This can be problematic for analytical studies based on the standard approach that assume a simple shape of Ω_{RE}

HOW TO COMPUTE THE PROBABILITY OF RUNAWAY P_{RE}?

- **Direct Monte-Carlo** [Fernandez-Gomez, et al.,Phys. Plasmas (2012)]. Straightforward to implement but inefficient and potentially inaccurate due to statistical sampling errors.
- **Adjoint Fokker-Planck** [Liu, et al., Phys. Plasmas (2016)]. Elegant and more efficient than the direct MC, but it requires the numerical solution of a PDE.
- **Backward-Monte Carlo** Based on the Feynman-Kac formula. Reduces the problem to the computation of Gaussian integrals. No MC sampling or PDE solving required! Efficient and unconditionally stable.
  - Zhang and del-Castillo-Negrete, Phys. Plasmas **24**, 092511 (2017)
  - Yang, Zhang, del-Castillo-Negrete, and Stoyanov, Journal of Comp. Phys **444**, 110564 (2021).

Feynman-Kac Formula

Intuitive description of simple 1D version

- Fokker-Planck equation

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\left[V(x)P(x,t)\right] + \frac{\partial^2}{\partial x^2}\left[D(x)P(x,t)\right] .$$

- Equivalent stochastic differential equation

$$dX = V(X)dt + \sqrt{2D(X)}\, dW(s)$$

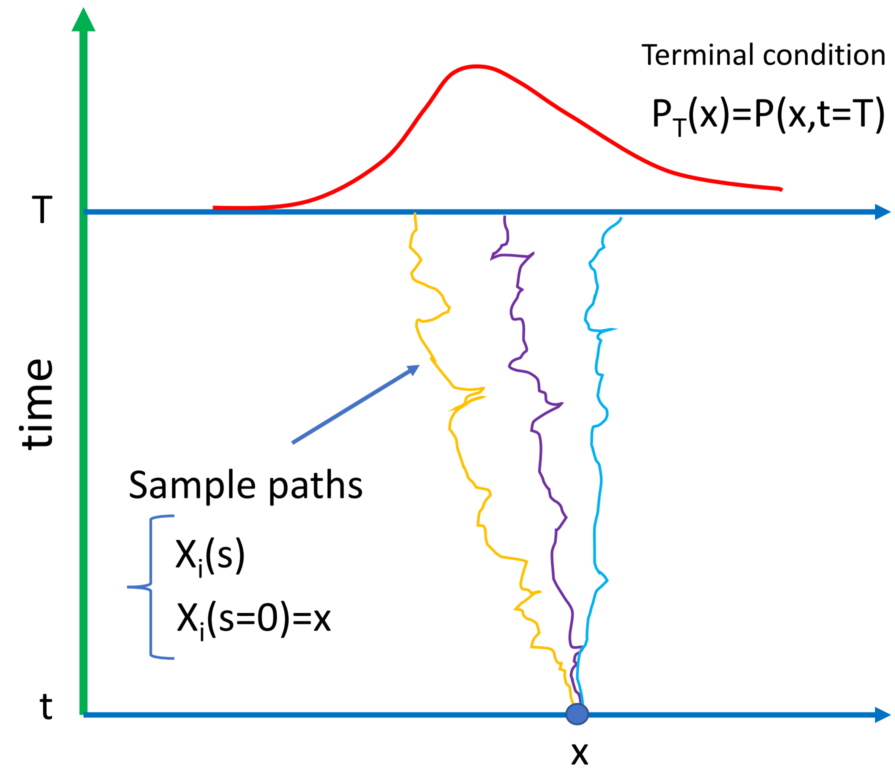
- Adjoint (Backward) Fokker-Planck equation

$$\frac{\partial P}{\partial t} + V(x)\frac{\partial P}{\partial x} + D(x)\frac{\partial^2 P}{\partial x^2} = 0$$

- The solution of the Backward Fokker-Planck equation with terminal condition $P(x, t = T) = P_T(x)$ is given by the Feynman-Kac formula:

$$P(x,t) = \mathbb{E}\left[P_T(X(T))|X(t) = x\right] \approx \frac{1}{N}\sum_{i=1}^{N} P_T(X_i(T))$$

where $\{X_i(t)\}$ are sample paths of the stochastic system such that $X_i(t) = x$, with $i = 1, \ldots N$, $N \gg 1$.



If interested in the extension and applications to nonlocal transport check my invited talk tomorrow

PROPOSED FEYNMAN-KAC BASED METHOD
(Simple version)

- To simplify the discussion, consider the following pitch angle, ξ, and momentum, p, Fokker-Plank model

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial p}(b_1 f) + \frac{\partial}{\partial \xi}(b_2 f) - \frac{1}{2}\frac{\partial^2}{\partial \xi^2}(\sigma^2 f) = 0$$

- In this case $P_{RE}(T-t, p, \xi) = P(t, p, \xi)$ where $P(t, p, \xi)$ is the solution of adjoint FP which according to the Feynman-Kac formula is given by the conditional expectation

$$P(t, p, \xi) = \mathbb{E}[\chi(p_T, \xi_T) \,|\, p_t = p, \xi_t = \xi]$$

$$\chi(p_T, \xi_T) = \begin{cases} 1, & \text{if } \ p_T \geq p_*, \\ 0, & \text{otherwise,} \end{cases}$$

where p_t and ξ_t are the paths of the stochastic equations

$$dp_t = b_1(p_t, \xi_t)\, dt,$$
$$d\xi_t = b_2(p_t, \xi_t)\, dt + \sigma(p_t, \xi_t)\, dW_t$$

DISCRETIZATION OF FEYNMAN-KAC FORMULA REDUCES THE COMPUTATION TO GAUSSIAN INTEGRALS

- Introduce a partion $\mathcal{T} = \{0 = t_0 < t_1 < \cdots < t_N = T\}$, of $[0, T]$, and for small $\Delta t = t_{n+1} - t_n$ approximate

$$\begin{aligned} p_{t_{n+1}} &\approx p_{t_n} + b_1(p_{t_n}, \xi)\,\Delta t \\ \xi_{t_{n+1}} &\approx \xi_{t_n} + b_2(p_{t_n}, \xi_{t_n})\,\Delta t + \sigma(p_{t_n}, \xi_{t_n})\,\Delta W, \end{aligned}$$

- Within the time interval $[t_n, t_{n+1}]$, write

$$P(t_n, p, \xi) = \mathbb{E}\left[P(t_{n+1}, p_{t_{n+1}}, \xi_{t_{n+1}}) \mid p_{t_n} = p, \xi_{t_n} = \xi\right].$$

  and, using the Gaussian propagator, approximate

$$P(t_n, p, \xi) \approx \int_{\mathbb{R}} P\left(t_{n+1}, p + b_1\Delta t, \xi + b_2\Delta t + \sigma x\right) \frac{e^{-\frac{1}{2}\frac{x^2}{\Delta t}}}{\sqrt{2\pi\Delta t}} dx\,,$$

  which can becomputed using Gauss-Hermite quadrature rules.
- Also, an interpolation in (ξ, p) space is needed at each step.

- Some advantages of the method
  - Unconditionally stable (no need to solve PDEs)
  - Second order convergence in space, first order in time
  - No need to sample orbit (no MC noise)
  - Straightforward to parallelize.

- Further details of the method, including:
  - GPU accelerated matrix representation implementation for time-dependent models, e.g. $T = T(t)$ and $E = E(t)$.
  - Use of piecewise cubic Hermite interpolating polynomials
  - 3D examples including applications to fluid mechanics
  - Benchmarks with analytical solutions and comparisons with explicit and implicit adjoint Fokker-Planck solvers

can be found in:

Journal of Computational Physics 444 (2021) 110564

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

ELSEVIER

A Feynman-Kac based numerical method for the exit time probability of a class of transport problems ☆

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RE generation problem

- As an integral part of the ASCR and OFES collaboration, with colleagues of the ORNL Applied Math group we developed the Backward Monte Carlo (BMC) code

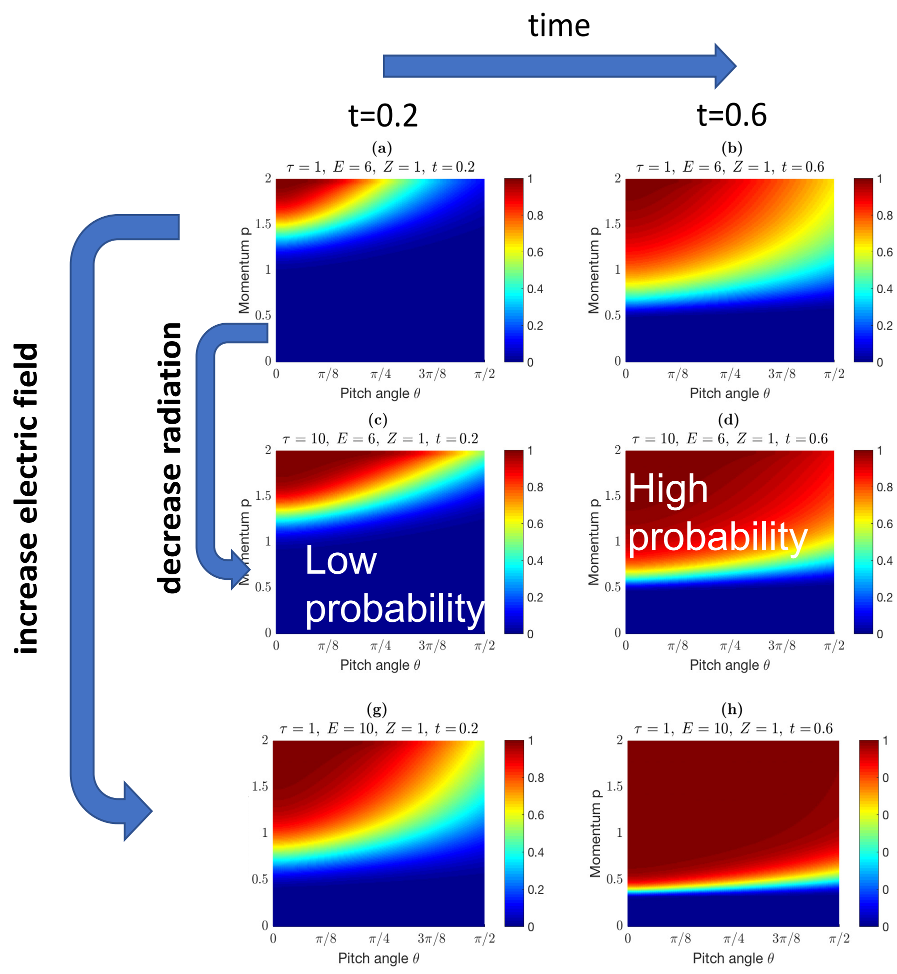
- The BMC is based on the Feynman-Kac formula and provides the probability of an electron to runaway given an initial condition and plasma state

- BMC is fully parallelizable, and allows the accurate and efficient evaluation of the dependence of the RE production rate on physical parameters and plasma states

- The current version of the algorithm has been extended to 3D fully time dependent regimes to study the role of confinement in dynamic thermal quench scenarios

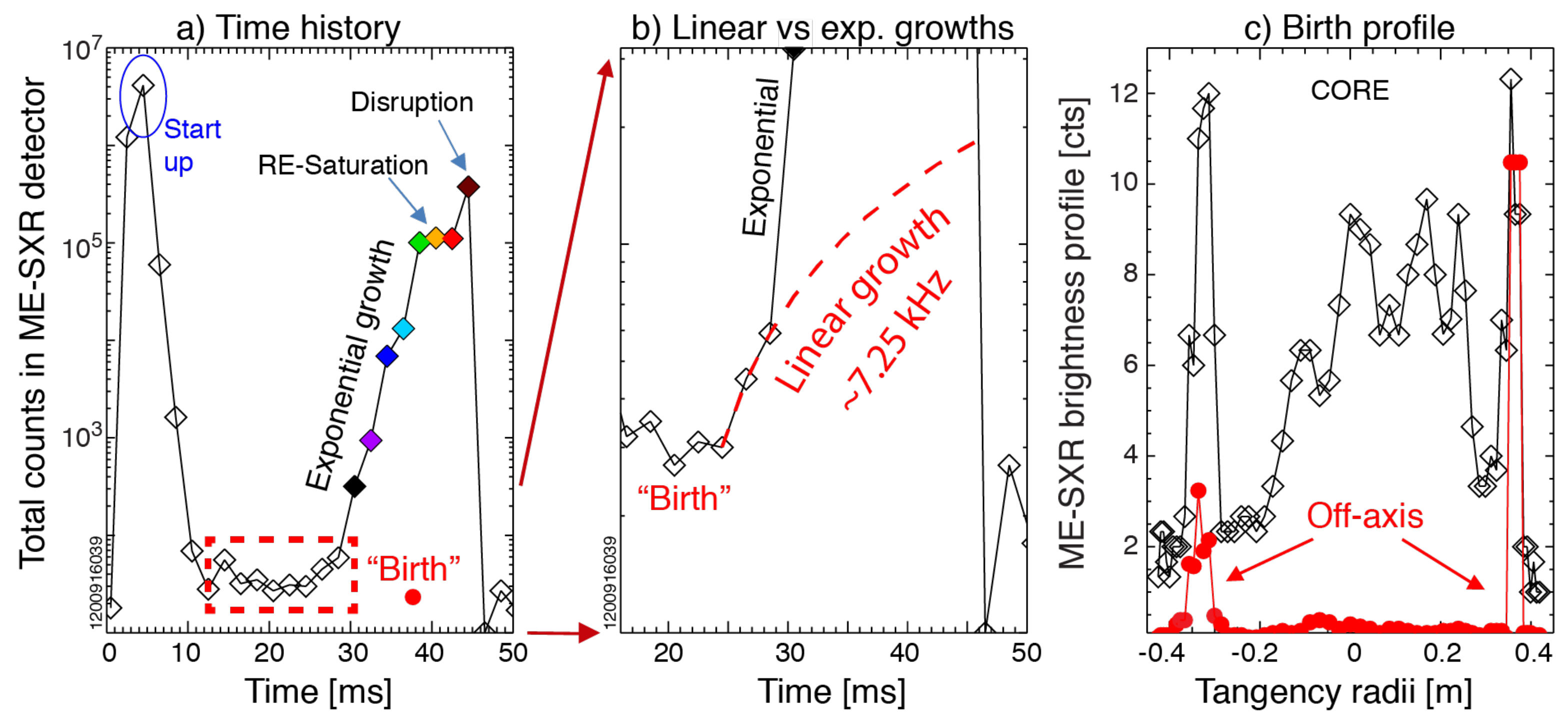
- We have also explored the use of BMC as an efficient method to couple the kinetic description of RE with the fluid description of the plasma

Fast and accurate exploration of a RE generation for different disruption scenarios



Seed RE observed during quiescence n_e ramp down regimes in MST

RE predominantly form at the edge



Delgado-Aparicio, et al Submitted to PRL (2022)
Invited Talk Wednesday 10:00 AM

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3D RUNAWAY ELECTRON ACCELERATION MODEL

3D+1 Fokker-Planck equation for $f(r, p, \xi; t)$

$$\frac{\partial f}{\partial t} = \mathcal{F} + \mathcal{R} + \mathcal{C} + \mathcal{D}\,, \qquad \text{with}$$

- Electric field force $\mathcal{F}\{f\} = -E\left[\xi\,\frac{\partial f}{\partial p} + \frac{(1-\xi^2)}{p}\frac{\partial f}{\partial \xi}\right]$
- Synchrotron radiation reaction force

$$\mathcal{R}\{f\} = \frac{1}{\tau}\left\{\frac{1}{p^2}\frac{\partial}{\partial p}\left[p^3\gamma\left(1-\xi^2\right)f\right] - \frac{\partial}{\partial \xi}\left[\frac{1}{\gamma}\xi\left(1-\xi^2\right)f\right]\right\}\,.$$

- Collision operator

$$\mathcal{C}\{f\} = \frac{1}{p^2}\frac{\partial}{\partial p}\left\{p^2\left[C_A\frac{\partial f}{\partial p} + C_F f\right]\right\} + \frac{C_B}{p^2}\frac{\partial}{\partial \xi}\left[\left(1-\xi^2\right)\frac{\partial f}{\partial \xi}\right]\,,$$

- Radial diffusion operator

$$\mathcal{D}\{f\} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD\frac{\partial f}{\partial r}\right]\,,$$

COLLISIONS MODEL

$$
\begin{aligned}
C_A(p) &= \bar{\nu}_{ee}\,\bar{v}_T^2\,\frac{\psi(x)}{x}\\
C_B(p) &= \frac{1}{2}\,\bar{\nu}_{ee}\,\bar{v}_T^2\,\frac{1}{x}\left[Z+\phi(x)-\psi(x)+\frac{\delta^4}{2}x^2\right]\\
C_F(p) &= 2\,\bar{\nu}_{ee}\,\bar{v}_T\,\psi(x)\,.
\end{aligned}
$$

where $x = \frac{1}{\bar{v}_T}\frac{p}{\gamma}\,, \qquad \gamma = \sqrt{1+\left(\tilde{\delta}p\right)^2}\,, \qquad \tilde{\delta} = \frac{\tilde{v}_T}{c} = \sqrt{\frac{2\tilde{T}}{mc^2}}$

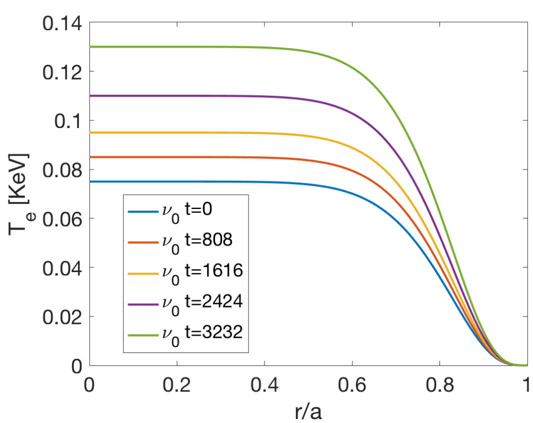
$$
\phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-s^2}ds\,, \qquad \psi(x) = \frac{1}{2x^2}\left[\phi(x) - x\frac{d\phi}{dx}\right]
$$

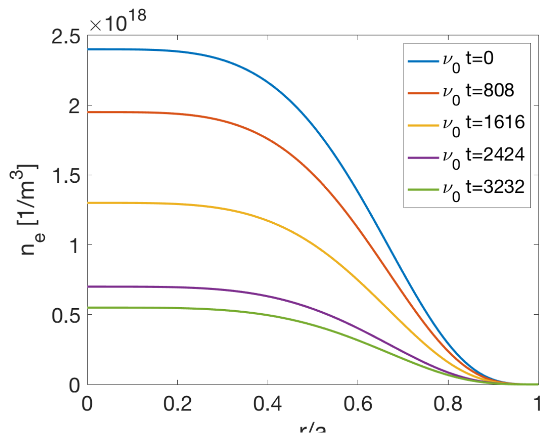
and the time dependence enters through the variables

$$
\bar{v}_T(t) = \sqrt{\frac{\hat{T}}{\tilde{T}}}\,, \qquad \bar{\nu}_{ee}(t) = \left(\frac{\tilde{T}}{\hat{T}}\right)^{3/2}\frac{\ln\hat{\Lambda}}{\ln\tilde{\Lambda}}\,, \qquad \delta(t) = \sqrt{\frac{2\hat{T}}{mc^2}}
$$

where $\hat{T}(t)$ denotes the time-dependent plasma temperature.

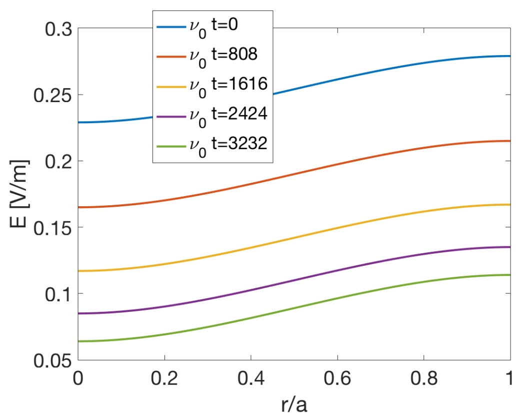
Spatiotemporal temperature, density and electric field models inferred from MST measurements

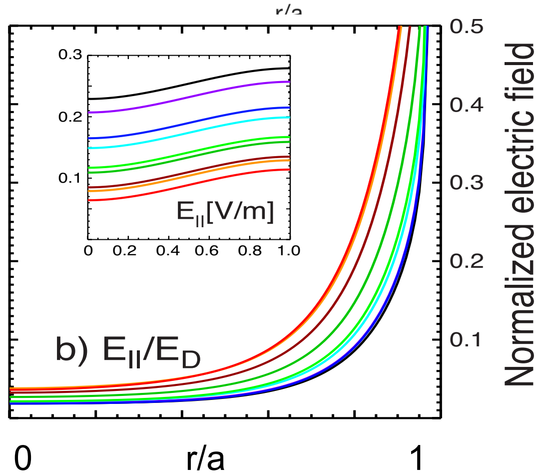




Dreicer critical electric field

$$\tilde{E}_D = \frac{\tilde{n} e^3 \ln \tilde{\Lambda}}{4\pi\epsilon_0^2 \tilde{T}}$$

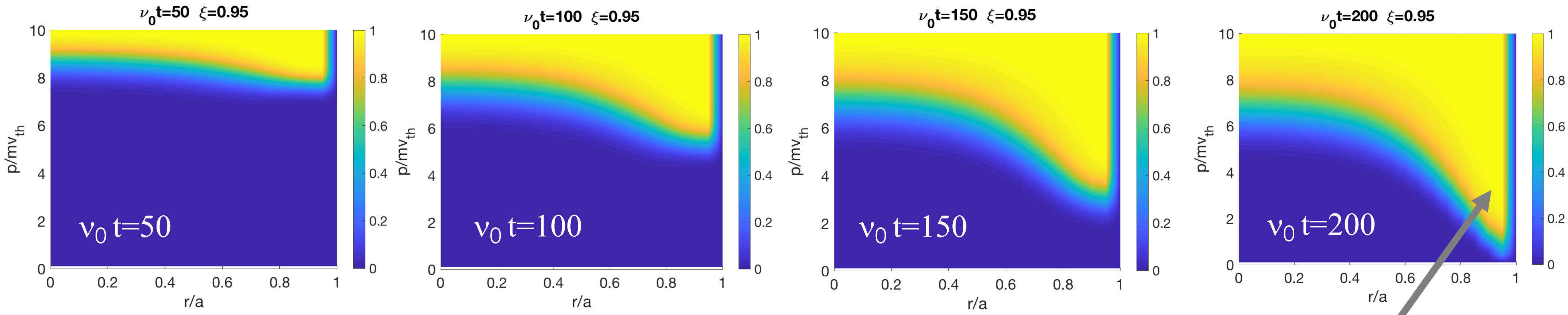




The density drop and the temperature rise at the at the edge lower the Dreicer field and promotes the creation of seed REs there

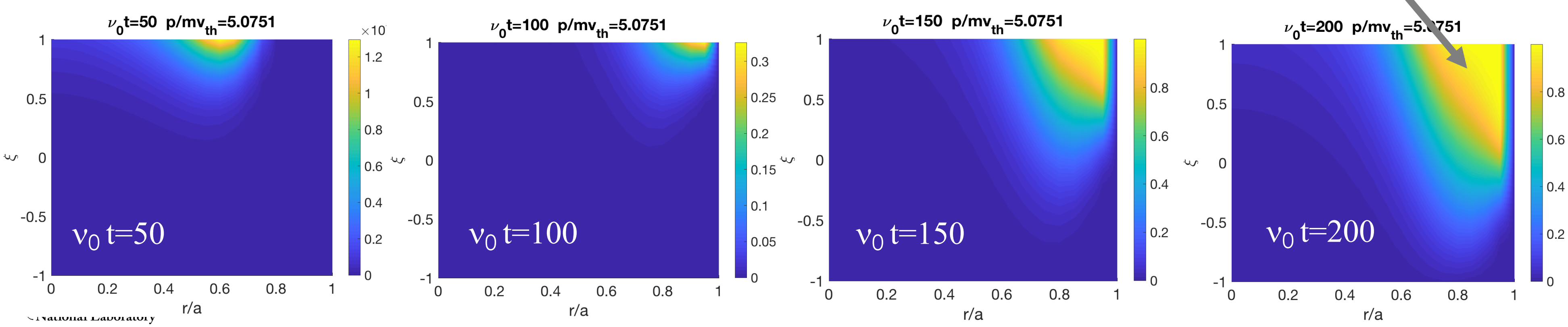
Dynamics of probability of runaway P_{RE} in 3D phase space

(p,r) space for fixed pitch angle ζ=0.95

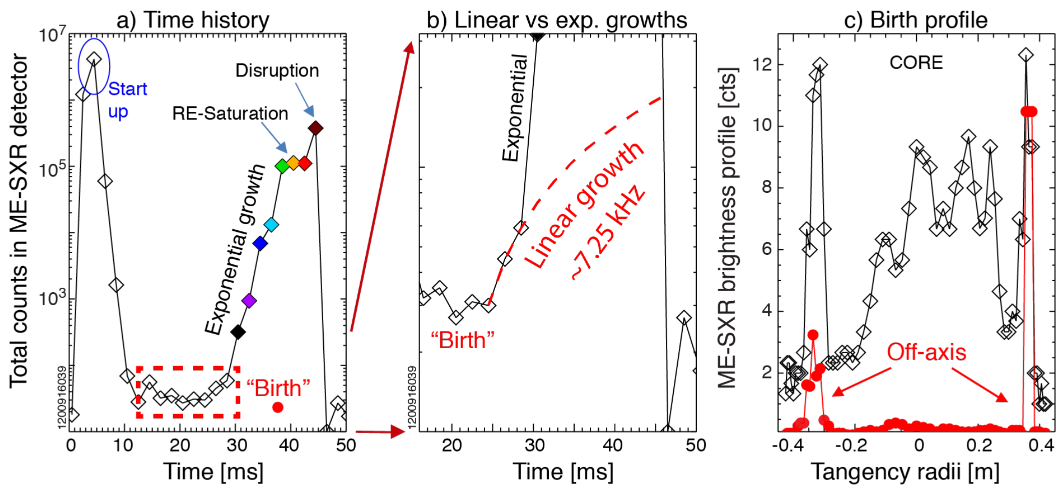


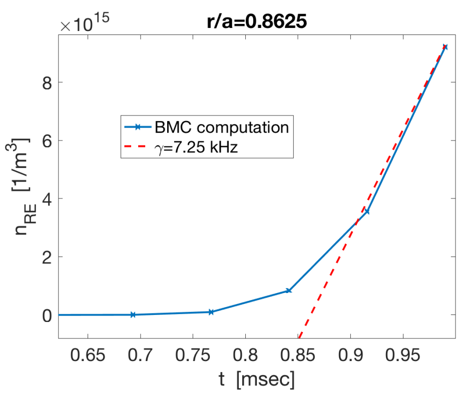
strong radial edge localization

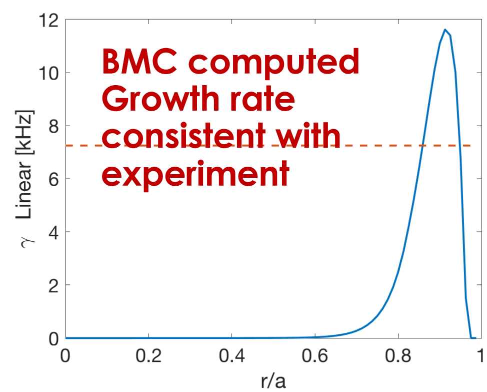
(ζ,r) space for fixed momentum p=5 m v_{th}

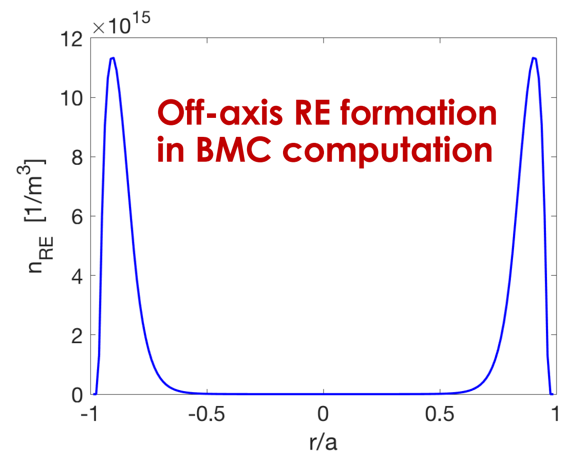


Quantitative agreement between BMC computations and MST observations



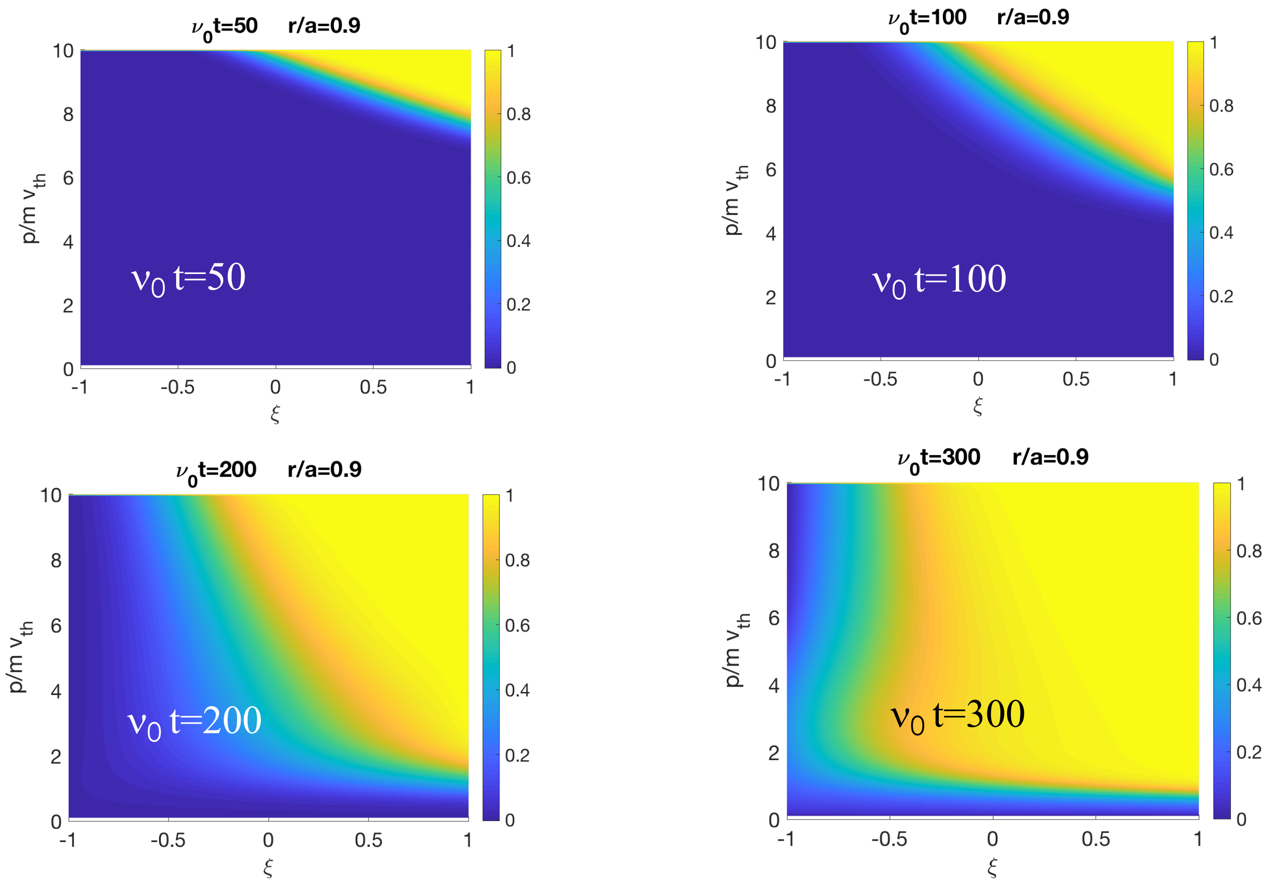






Dynamics of probability of runaway P_{RE} in 3D phase space

(ζ ,p) space at the edge r/a=0.9



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A heuristic model to describe the density peaking

$$\frac{\partial u}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_r) + \gamma u + S$$

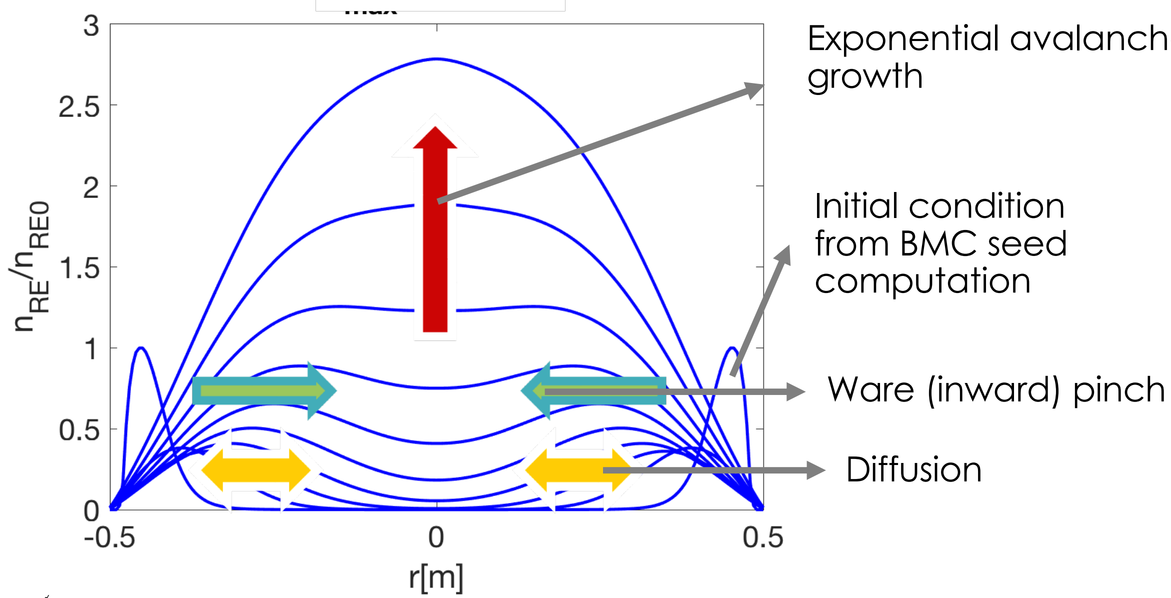
where the flux, Γ_r is defined in cylindrical coordinates as

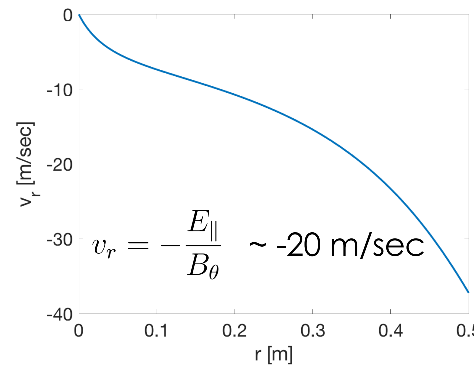
$$\Gamma_r = v_r u - D\frac{\partial u}{\partial r},$$

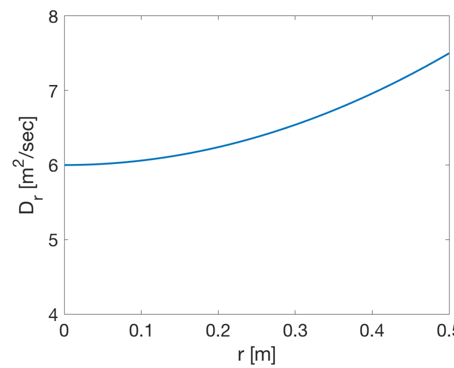
γ is the avalanche growth rate, and S the source.

- Seed RE at the edge avalanche
- Fraction of new RE are trapped
- Trapped RE transported by Ware pinch
- As RE drift to the core they are de-trapped

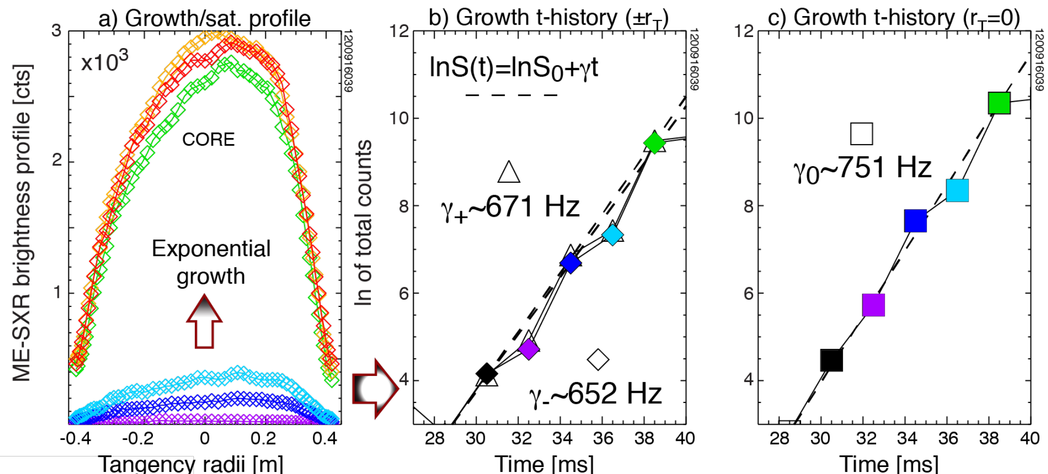
[Nilsson et al., J. Plasma Phys (2015)]

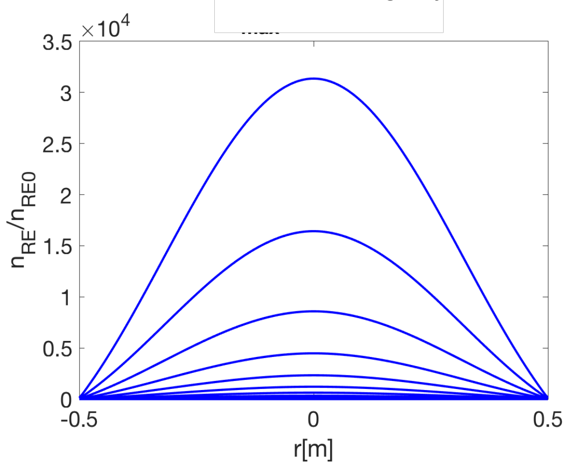


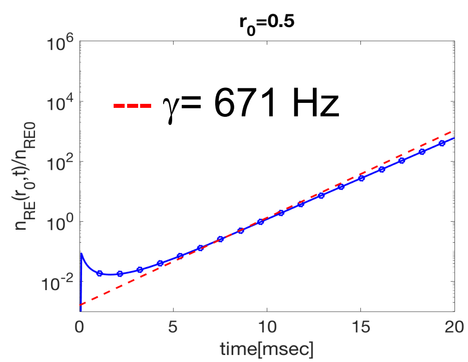


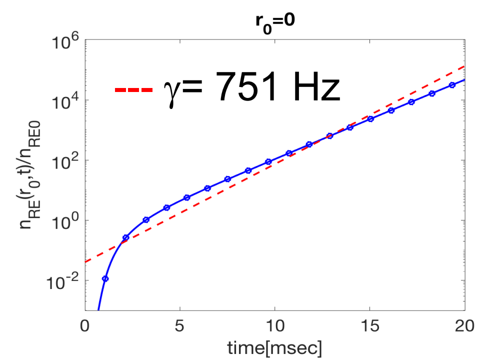


Good qualitative agreement between heuristic model and MST observations







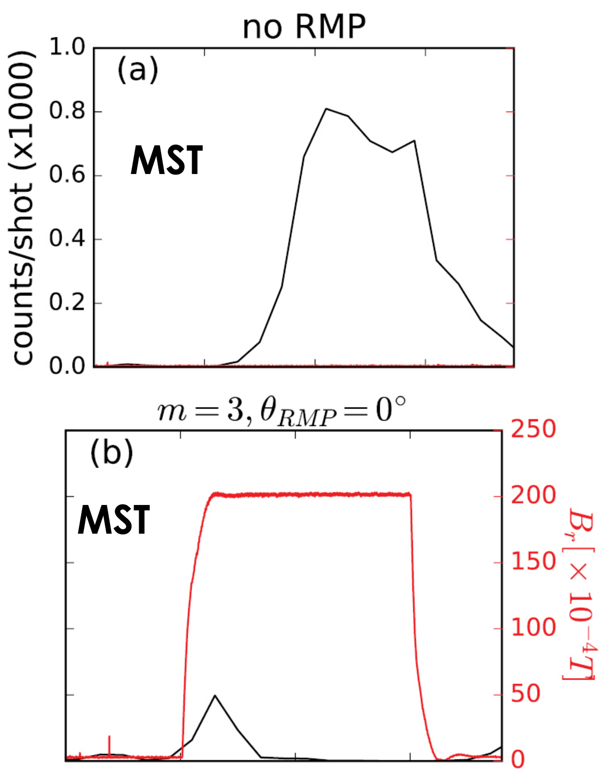


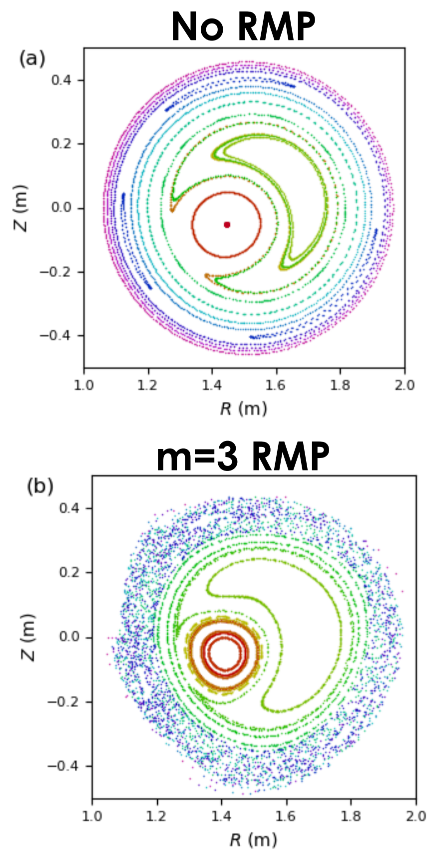
RE avoidance problem:

NIMROD + KORC modeling of RE suppression in MST using RMPs

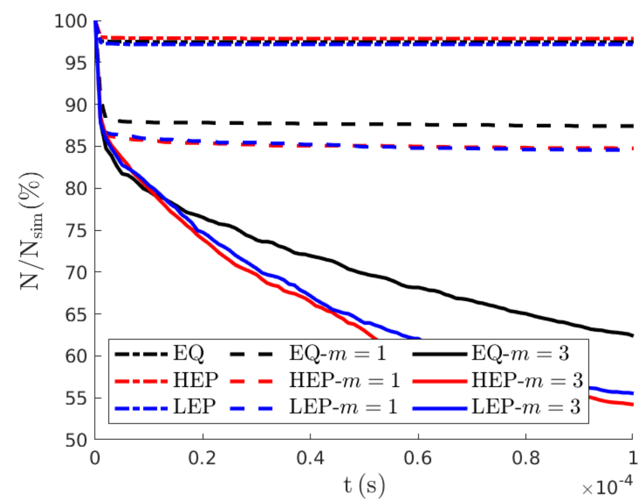
S. Munaretto et al., Nuclear Fusion 60, 046024 (2020)

B. Cornille et al. Phys. Plasmas (2022).





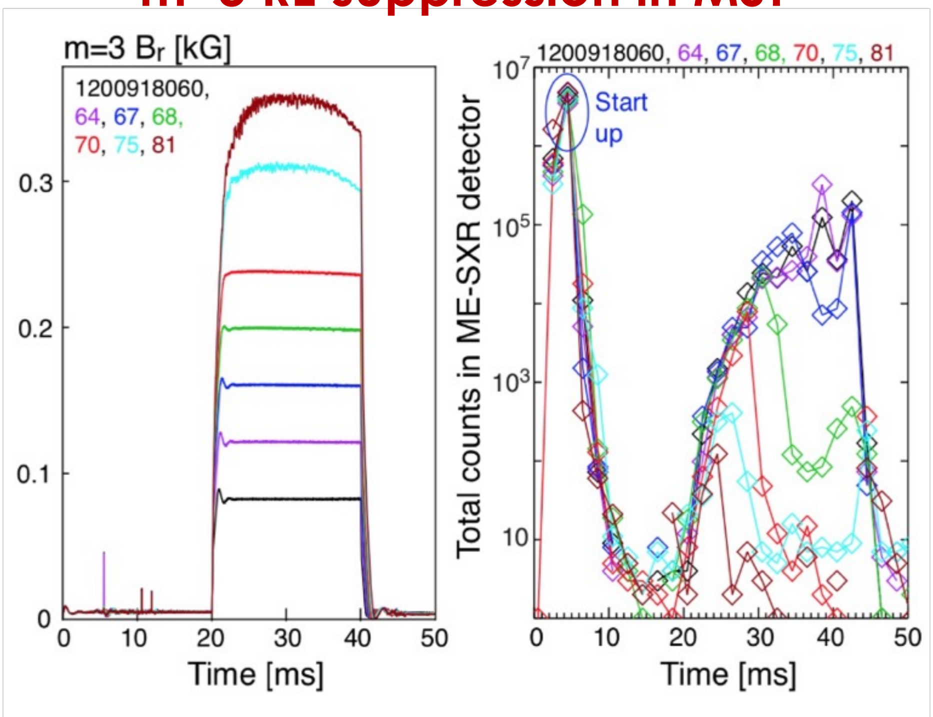
In **agreement with the experiment** NIMROD + KORC simulations show RE **deconfinement with m=3 but not with m=1**



However, contrary to the experiment, **total RE loss not observed**

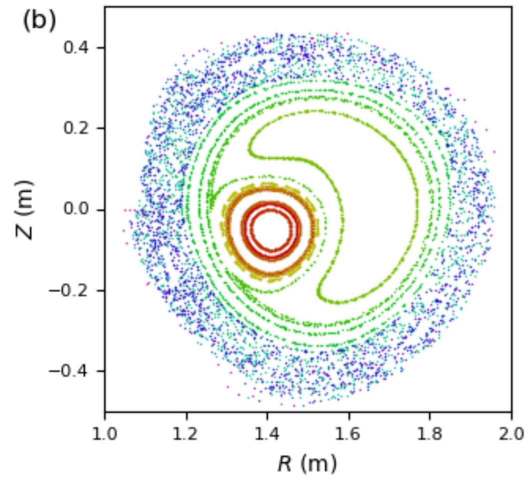
Modeling of RMP suppression of RE using BMC

m=3 RE suppression in MST

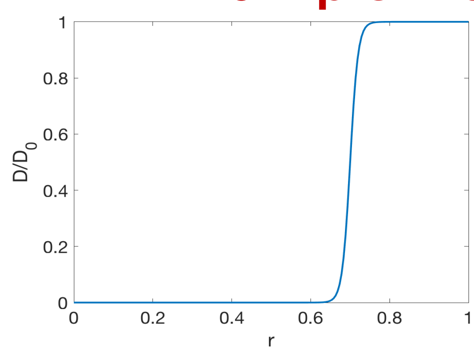


Delgado-Aparicio, et al Submitted to PRL (2022) Invited Talk Wed 10:00 AM

m=3 B field stochasticity in NIMROD



Simple model in BMC



$$D_r = \frac{D_0}{2}\left\{1+\tanh\left[\frac{r-r_D}{L_D}\right]\right\}$$

$$D_0 \sim (\delta B / B)^2$$

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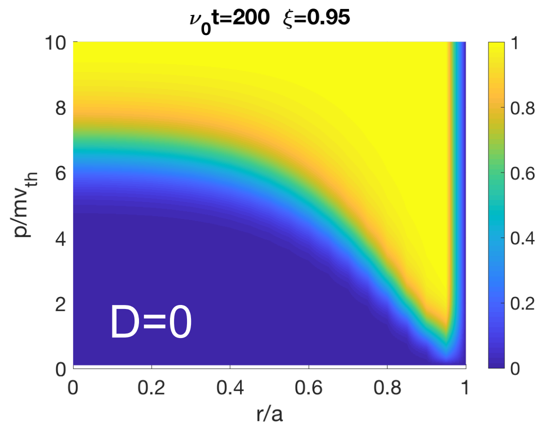
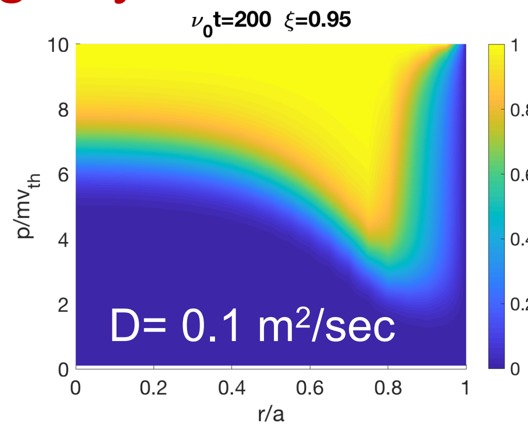
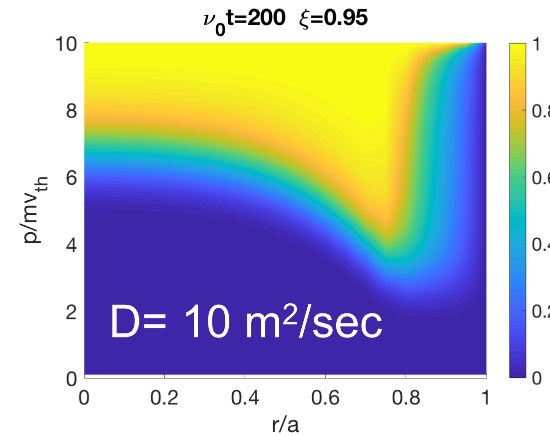
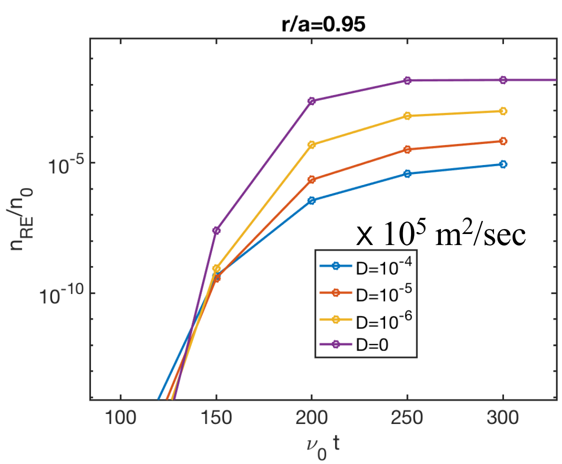
Modeling of RMP suppression of RE using BMC

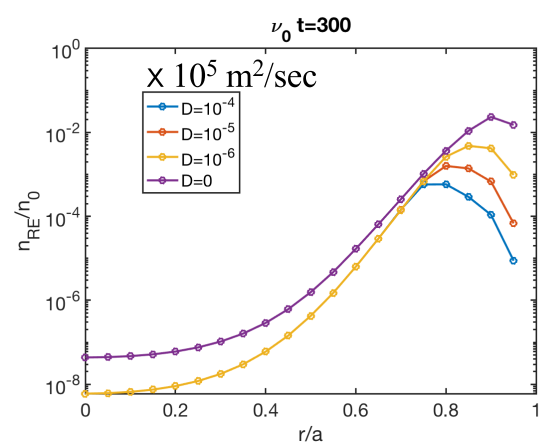
(p,r) space for fixed pitch angle $\zeta=0.95$











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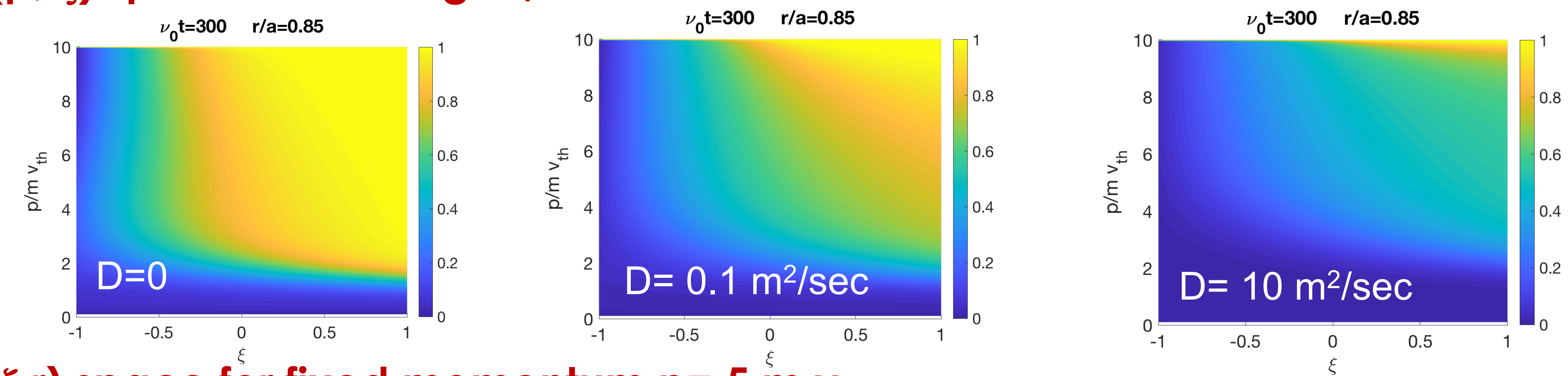
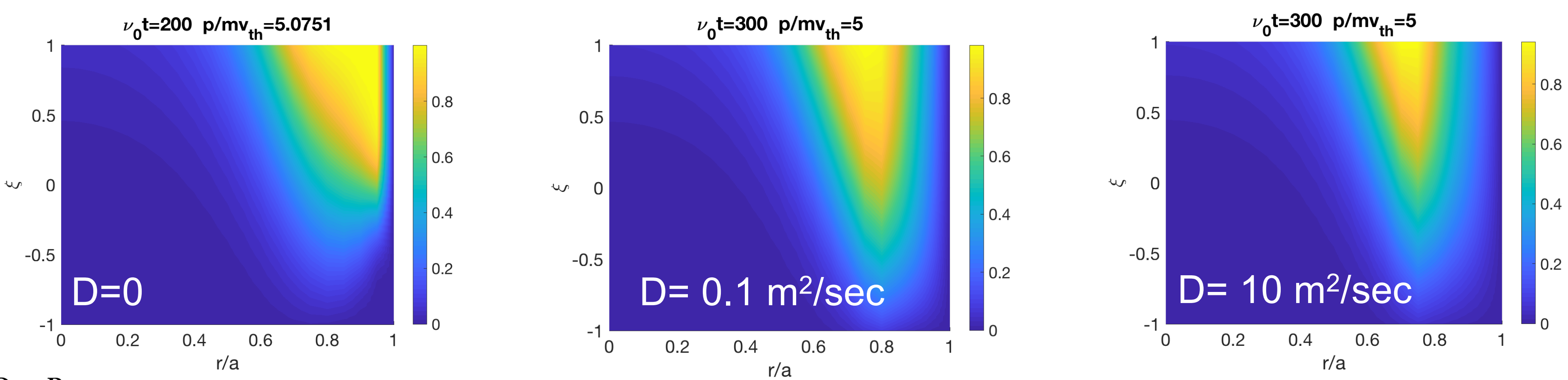
Modeling of RMP suppression of RE using BMC

(p, ζ) space at the edge r/a=0.95



(ζ,r) space for fixed momentum p= 5 m v_{th}



Modeling of RE generation in thermal quenched plasmas

- Rechester-Rosenbluth type radial diffusion model

$$D = \hat{D}_0\, F(r) G(p)\,, \qquad \hat{D}_0 = \pi q v_{\|} R \left(\frac{\delta B}{B}\right)^2\,,$$

with spatial and momentum dependence

$$F(r) = \frac{1}{2}\left\{1 + \tanh\left[\frac{r - r_D}{L_D}\right]\right\}\,, \qquad G(p) = e^{-(p/\Delta p)^2}\,.$$

- Exponential cooling model with thermal quench time scale t_*

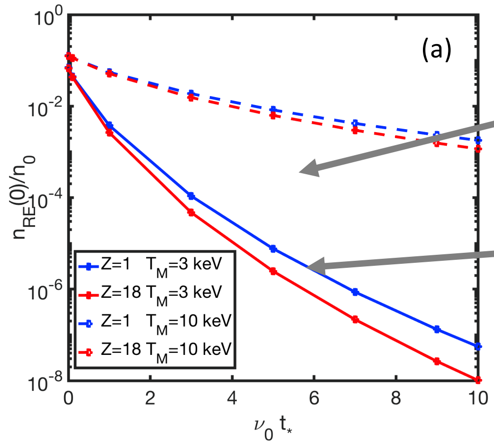
$$\hat{T} = \hat{T}_f + \left(\hat{T}_0 - \hat{T}_f\right) e^{-t/t_*}\,,$$

- Electric field dependence from Ohms's law and Spitzer conductivity

$$E(t) = E_0 \left[\frac{\hat{T}_0}{\hat{T}(t)}\right]^{3/2}\,.$$

RE generation problem: Dependence on thermal quench time scale

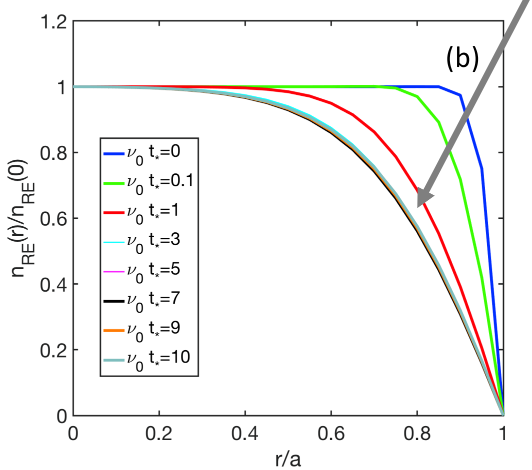
3D time-dependent BMC simulations

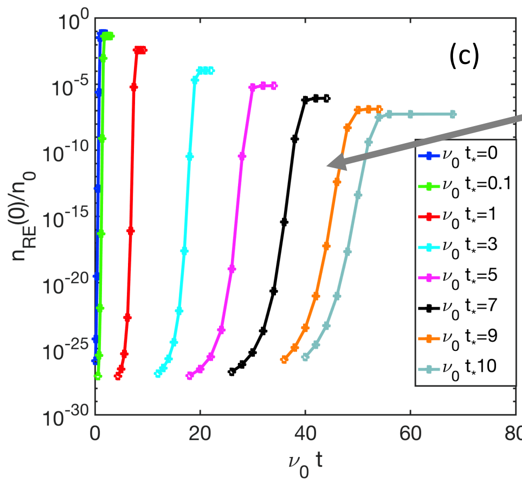


Seed RE production has a **strong dependence on thermal quench time** and initial temperature

There is a **weaker dependence on Z**

Diffusion reduces the gradient of the radial seed density profile at the edge and this effect increases with the termal quench time



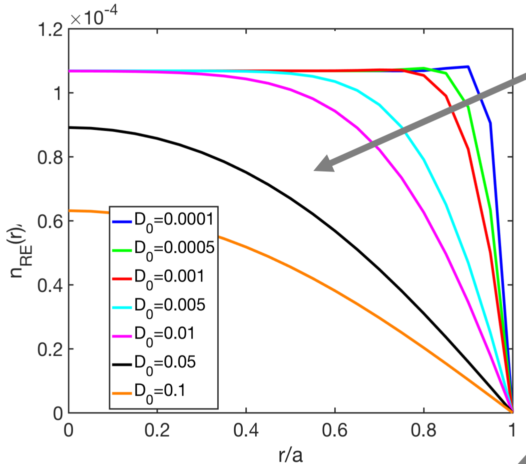


The onset of the **saturation of the seed runaway** is significantly affected by the thermal quench time scale

D. del-Castillo-Negrete, et al., *28th IAEA Conference*.(2021) IAEA-CN-286/101.

RE generation problem: Dependence on radial diffusive transport

3D time-dependent BMC simulations

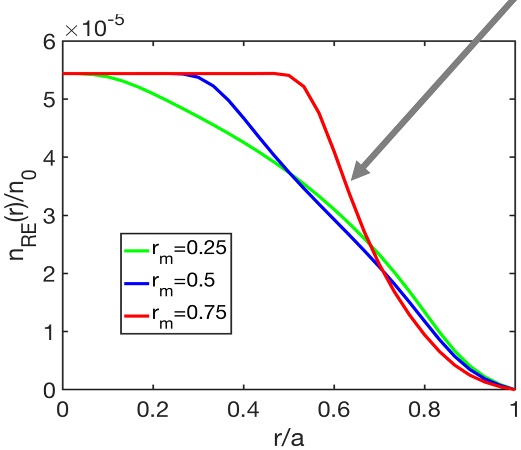


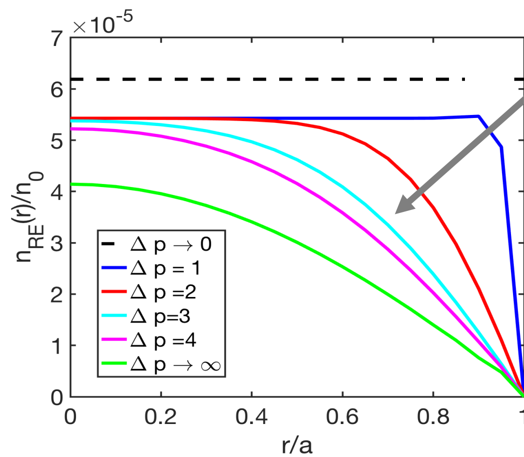
RE seed production decreases when D_0 (normalized by 10^4 m^2/s) *increases and this effect is stronger at the edge*

Model for spatial and mometum dependent diffusivity:

$$D(r,p) = \frac{D_0}{2}\left\{1 + \tanh\left[\frac{r - r_m}{L_D}\right]\right\} e^{-(p/\Delta p)^2}$$

Location r_m of diffusive transport barriers leads to pedestal in RE production rate profile





High momentum suppression of diffusive transport introduce momentum dependent production rate radial profiles

D. del-Castillo-Negrete, et al., *28th IAEA Conference*.(2021) IAEA-CN-286/101.