RF operator in RFMC Monte Carlo code (and other updates)

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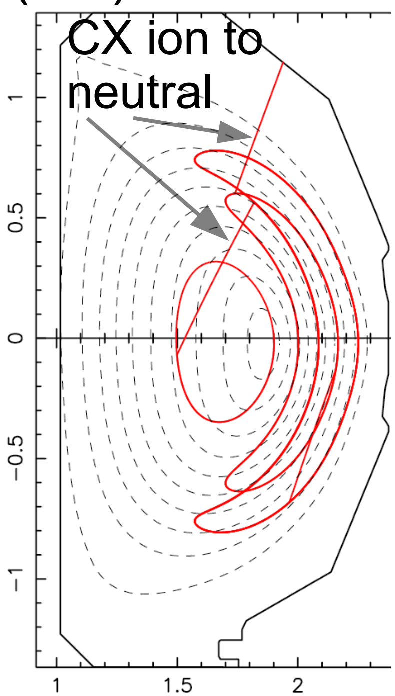
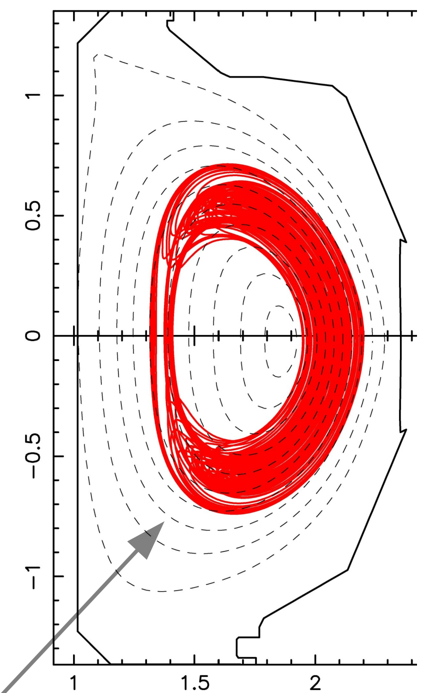
Main Features and Goals

- Cross-verification of CQL3D.
- Provide an RF-SciDAC Monte Carlo 5/6D calculation of ion distributions subject to RF and NB heating, for general DOE computing systems.
- Treat non-axisymmetric features including losses to PFCs (including the wall).
- RFMC derives from MCGO (www.compxco.com/mcgo.html)

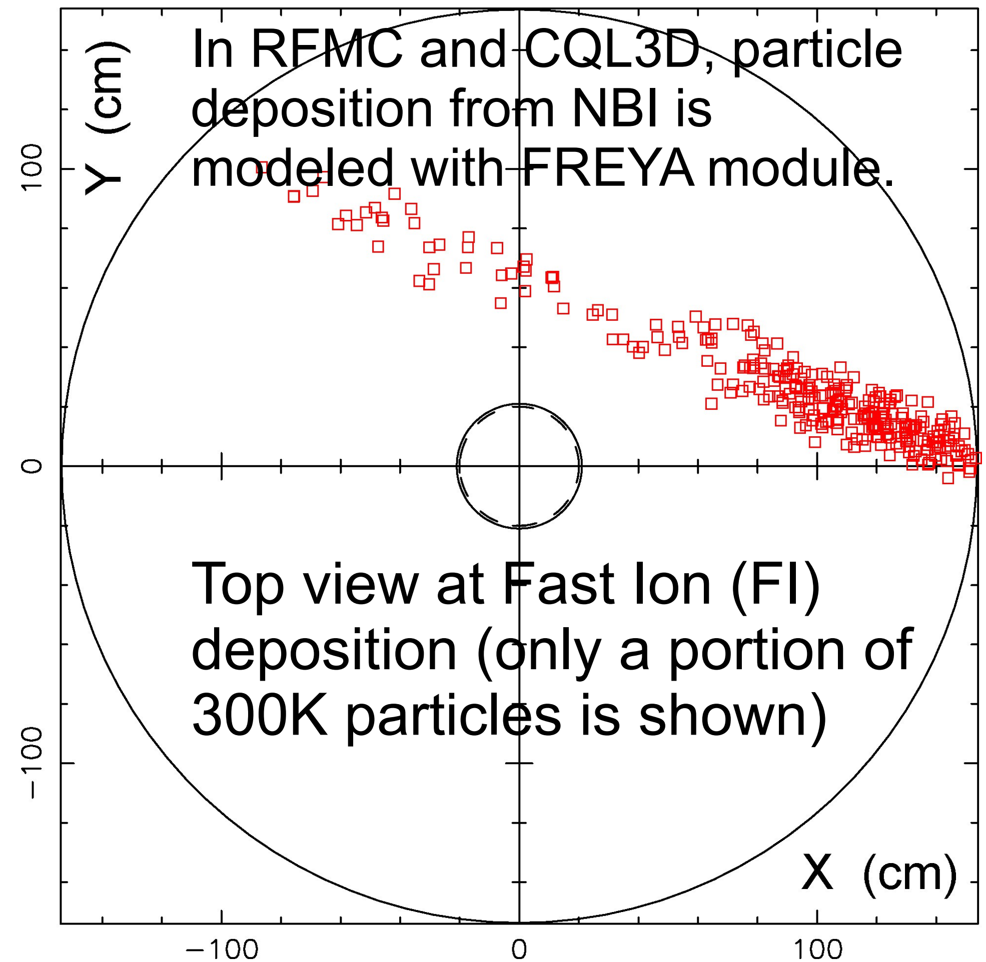
Fast ions can charge-exchange (CX) to neutrals.



Collisions with background e and ions:



Initially trapped ion (D+ at 70 keV): 107 bounce periods or transits, 35ms of phys. time.



Main Features

- GC, GC+gyro-correction (5D), and full orbits (6D)
- Background plasma profiles specified (tabulated+spline)
- Profiles of neutrals – used for modeling of CX events
- Equilibrium B-field – from EQDSK
- Multi-species beams – FREYA module for fast ion deposition
- Combined NBI+Maxwellian group loading
- Coulomb collisions (pitch angle, slowing, energy diffusion)
- "Goosing" for orbit speedup (accelerated collisions → faster slowing-down in energy; applied when t_bounce << t_coll)
- Distribution function (vel. space) is formed at the midplane radial bins
- Restart capabilities

Recently added:

- MPI
- RF diffusion (based on E_{rf} fields from full-wave Aorsa)
- Accumulation of lost particles over 4D grid – { length_along_limiter; particle_speed_at_impact; incident_angle; tor.angle_at_impact }
- Time frames for data accumulation → profiles(r,t)

RF kick operators

Three versions – all based on RF fields from AORSA (or TORIC)

iRFver=1 Solve $du_\perp/dt + i\Omega_c(t)u_\perp = \frac{q}{m}E_+\exp(-i\omega t) + \frac{q}{m}E_-\exp(+i\omega t)$

The change in perp. velocity $u_\perp$ is computed at <u>each</u> time step ($t_1 \rightarrow t_2$)

and E_- term

$$u_\perp(t_2) = \frac{u_\perp(t_1) + \int_{t_1}^{t_2} \frac{q}{m}E_+\exp\left(-i\omega\tilde{t} + iN_\phi\phi(\tilde{t})\right)\left[\exp\left(i\int_{t_1}^{\tilde{t}}\Omega_c\,d\tau\right)\right]d\tilde{t}}{\exp\left(i\int_{t_1}^{t_2}\Omega_c\,dt\right)}$$

Complex-value velocity (with gyro-phase) before and after one t-steps along the g.c. orbit ($t_2 = t_1 + \Delta t$).

Different from DC-fast code: In the MC code, the change in $u_\perp$ is applied at <u>every</u> step. In DC - after one poloidal transit for a bounce-aver formulation.

- Limitation on time step, because the integral has a quickly-oscillating kernel ~ exp($-i(\omega_{rf} - \Omega_c)$), when not near resonance.
- ~10x slower than iRFver=3 (next page).

iRFver=2 is same as above, but Ω_c is expanded around resonance and the integrals are evaluated (as in Stix_NF_1975). No E_- in this version, no finite $k_\perp\rho_{larm}$ effects, no high-harmonic interaction!

For both versions: What is a valid method for gyro-phase randomization?

iRFver=3 Based on local QL diffusion coefficients

Derivation is done in analogy with [X.Q. Xu and M.N. Rosenbluth, Phys.Fluids B **3**, 627 (1991)] for collision operator.

The kicks in $\Delta(V_\perp^2)$ and $\Delta V_{||}$ are given by these two equations

$$\Delta(V_\perp^2) = (\nu_{s\perp} V^2)\Delta t + 2\sqrt{3}(R_s - 0.5)\sqrt{(8 D_\perp V_\perp^2 \Delta t)}$$

$$\Delta V_{||} = (\nu_{s||} V_{||})\Delta t + 2\sqrt{3}(R_s - 0.5)\sqrt{(2 D_{||} \Delta t)}$$

where $$(\nu_{s\perp} V^2) = \frac{\partial(4\mathrm{D}_\perp V_\perp^2)}{\partial(V_\perp^2)} + \frac{\partial(2\mathrm{D}_{||\perp} V_\perp)}{\partial V_{||}}$$

and $$(\nu_{s||} V_{||}) = \frac{\partial D_{||\perp}}{\partial V_\perp} + \frac{\partial D_{||}}{\partial V_{||}} + \frac{D_{||\perp}}{V_\perp}$$

R_s is from uniform random distribution in [0; 1). It is the <u>same</u> number for both $\Delta(V_\perp^2)$ and $\Delta V_{||}$ kicks (in collision operator, they are different).

It can be shown that these kicks satisfy

$$\Delta(V_\perp^2) + 2(V_{||} - \omega/k_{||})\Delta V_{||} = 0$$ consistent with

$$V_\perp^2 + (V_{||} - \omega/k_{||})^2 = const$$ [Stix_NF_1975]

The local QL diffusion coefficients are

$$D_{\perp} = \frac{\pi q^2}{2m^2} |\theta_n|^2 \left(\frac{n\Omega_c}{\omega}\right)^2 \delta(\omega - k_{\|} V_{\|} - n\Omega_c)$$

$$D_{\|} = \frac{\pi q^2}{2m^2} |\theta_n|^2 \left(\frac{k_{\|} V_{\perp}}{\omega}\right)^2 \delta(\omega - k_{\|} V_{\|} - n\Omega_c)$$

and $D_{\|\perp}^2 = D_{\|} D_{\perp}$

where $\theta_n = E_+ J_{n-1} + E_- J_{n+1} + (V_{\|}/V_{\perp}) E_{\|} J_n$

and $J_n = J_n(k_{\perp} \rho_{larm})$ $k_{\perp}$ is not available from AORSA !

The kicks are applied at several steps before and after the resonance. Consider the wave-particle "interaction time" [based on Kerbel, McCoy, Phys. Fluids **28** (1985)], whichever is smaller:

$$t_{corr} = \sqrt{2\pi / \left| d(n\Omega_c)/dt \right|} \quad \text{or} \quad t_{corr} = 2\pi A_i(0) / \left| d^2(n\Omega_c)/dt^2 \right|^{1/3}$$

The delta-function is averaged over [$t_{\text{res}} - t_{\text{c}}$; $t_{\text{res}} + t_{\text{c}}$]

$$\frac{1}{2t_c} \int \delta(\omega - n\Omega_c - k_{\|} V_{\|}) = \frac{1}{2t_c} \frac{1}{\left| d(n\Omega_c)/dt \right|} = \frac{t_{corr}^2}{4\pi t_c}$$

In the code, we choose $t_{\text{c}} = t_{\text{corr}}$ (smaller value of t_{c} gives larger factor in the t_{c}-averaged $D_{\perp}$, but fewer number of kicks). Usually t_{c} is much larger than the orbital time step Δt , so the code makes several kicks around resonance.

The results are almost independent on the orbital time step Δt !

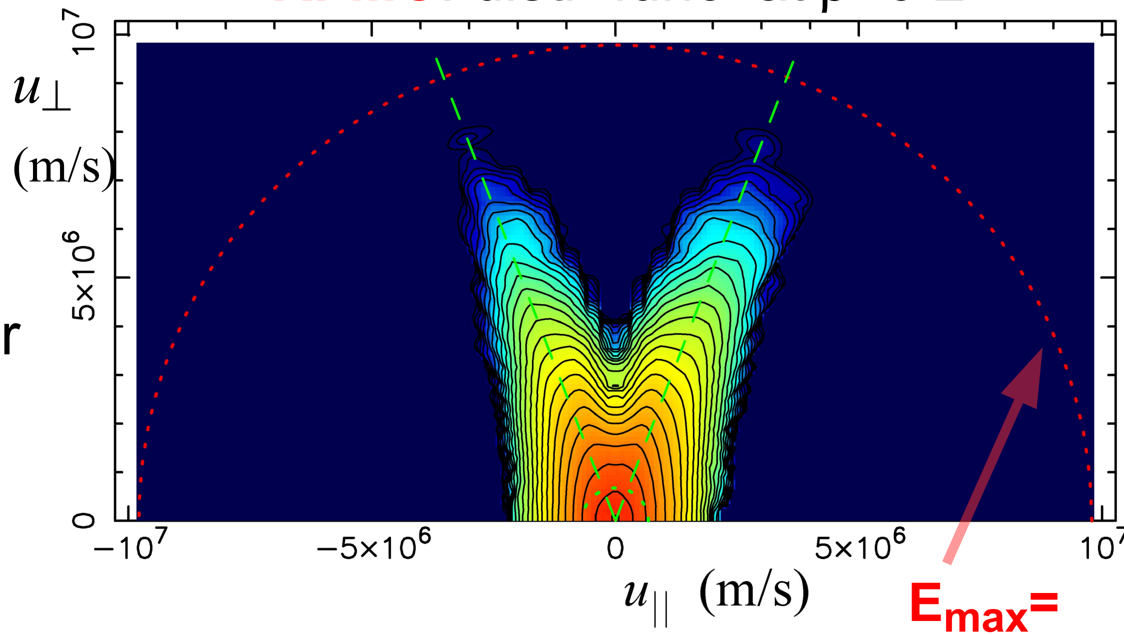
RF operator (iRFver=3): ICRH in C-Mod. RFMC vs CQL3D-ZOW

In RFMC run:

- 1 Million test ions.
- RF field is imported from AORSA run (4 toroidal modes used).
- The shown distribution is evaluated at the outer midplane position at R=73cm (ρ=0.2), not far from the ICR layer, which goes through the magnetic axis at R~68cm.
- tcpu=82sec on 480 cores on NERSC/Edison [compare to 52sec in no-RF run].
- Particles are followed up to t=1.5ms of physical time. 178M total crossings of the midplane.

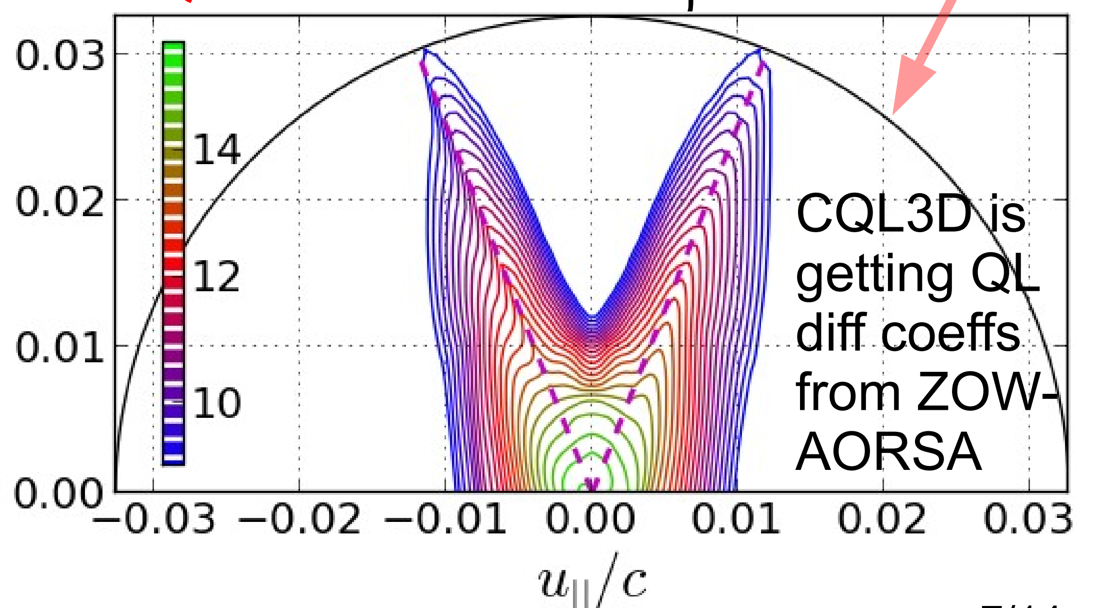
In RFMC run, the distribution is collected in t= [0.5; 1.5] ms range.
In CQL3D, the solution is at t=1ms (with accuracy of dt=0.05ms).
Not a Steady-State !

RFMC: distr. func. at ρ=0.2



E_{max}= 500keV

CQL3D: distr. func. at ρ=0.2

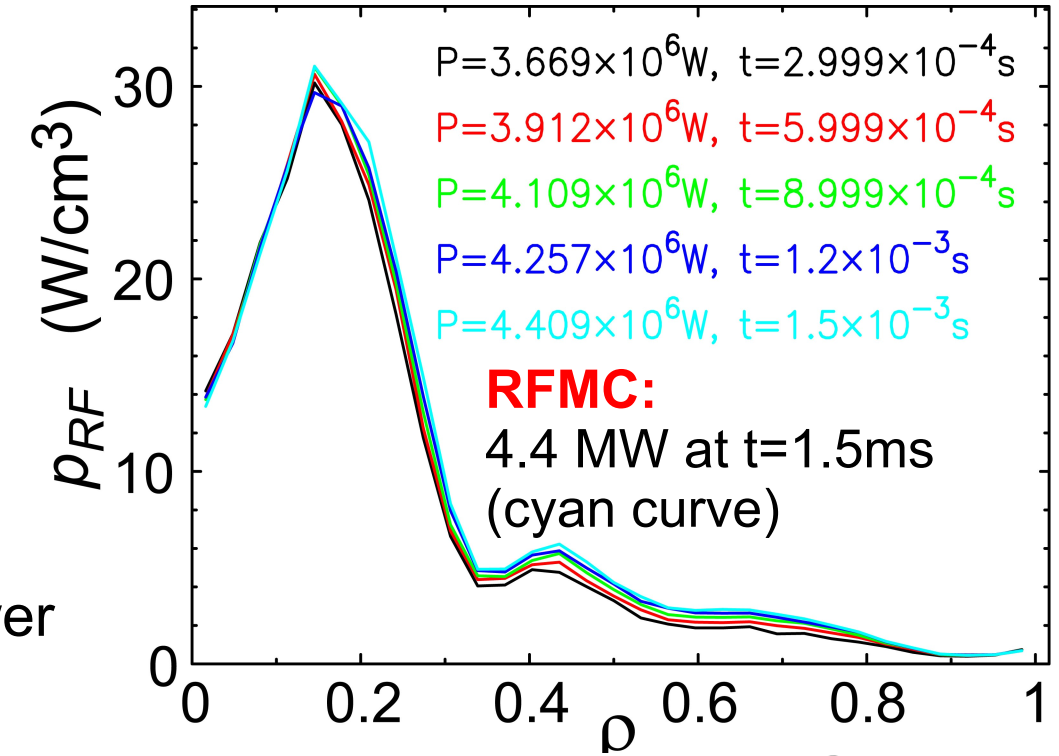


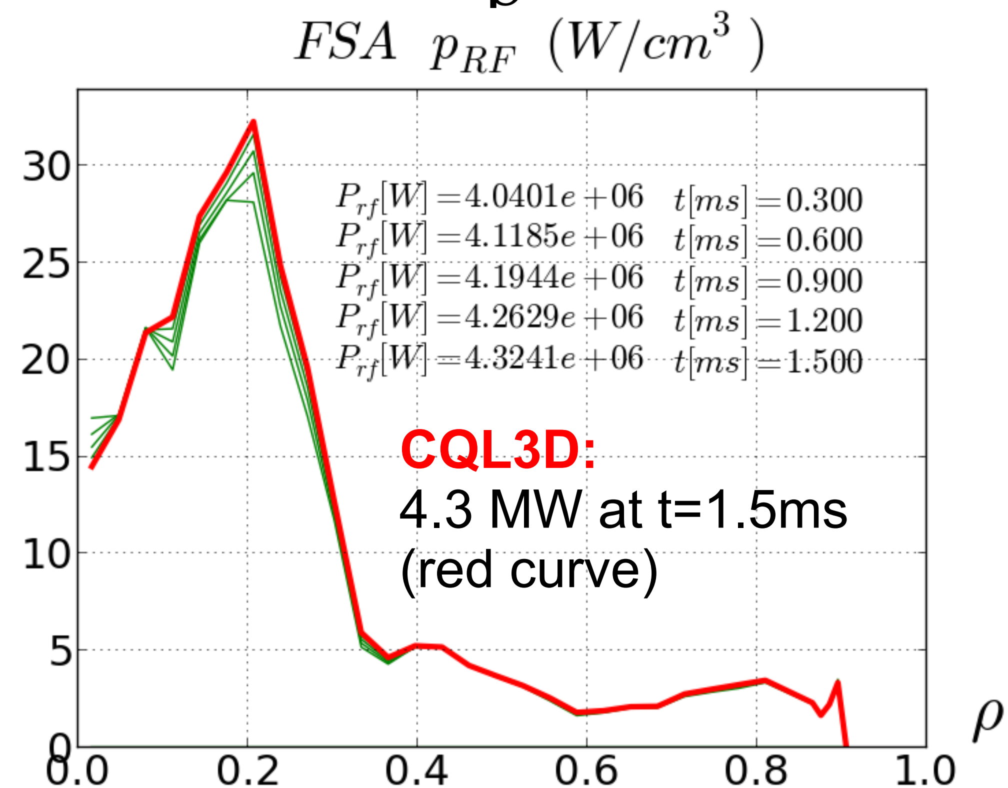
...cont-ed: ICRH in C-Mod. RFMC vs CQL3D-ZOW

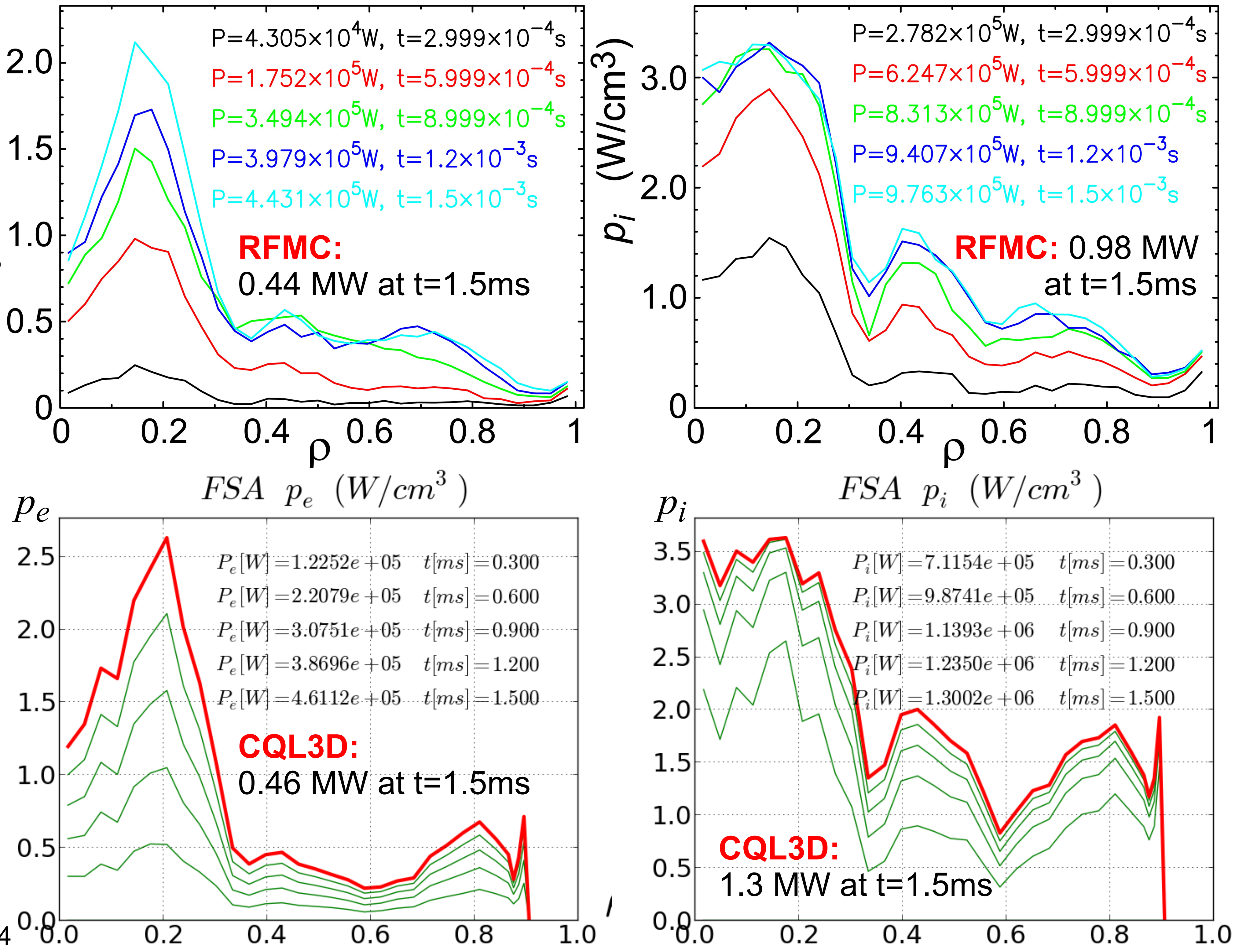
This slide: RF power deposition to H ions (minority heating).

Next slide shows collisional power transfer from H^+ minority ions to background electrons and ions (D^+).

In RFMC run, profiles are collected over time frames. The value of *t* specified in plots gives the ending time of each frame; the beginning time is at previous line.
In CQL3D run, data was saved at 30 steps, only five are plotted.





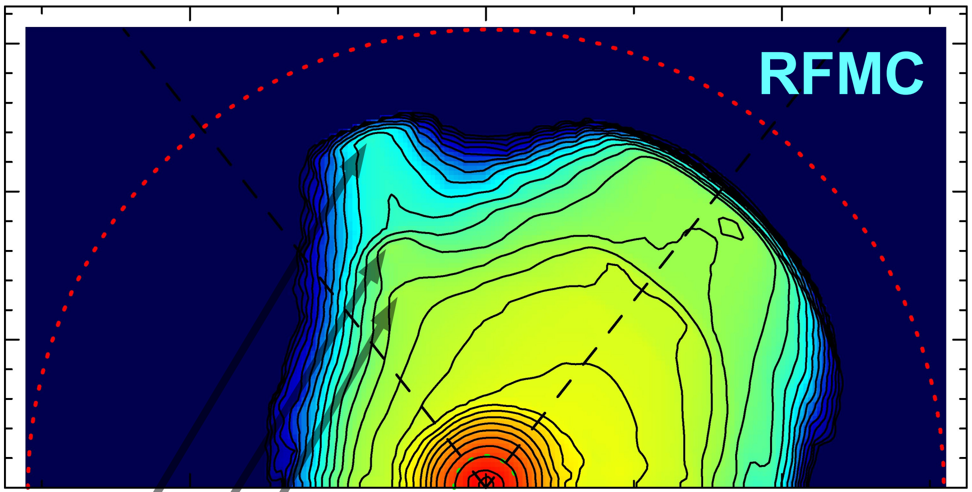


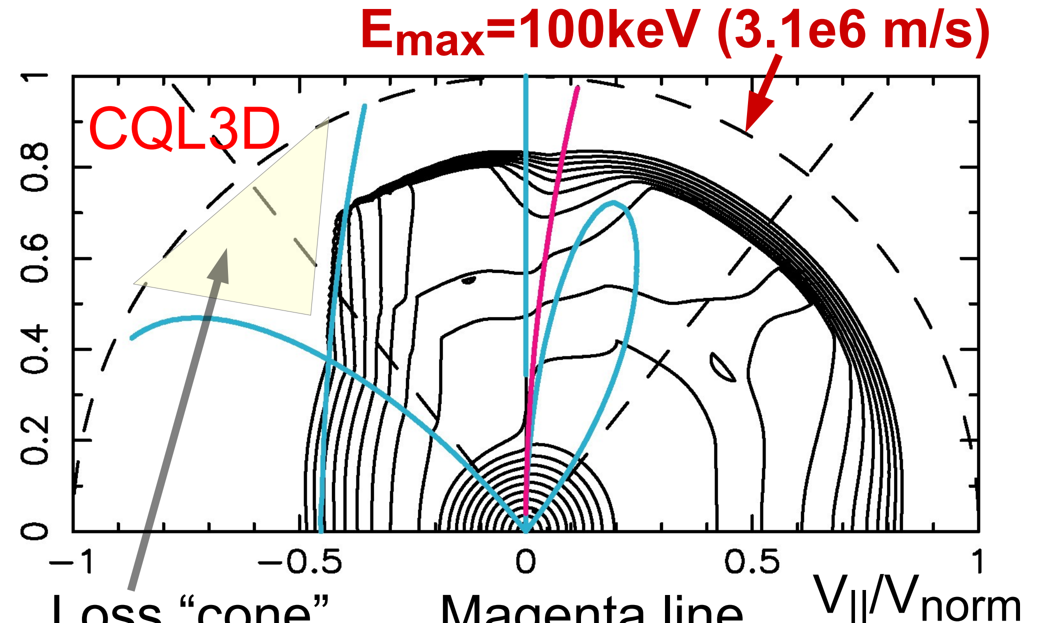
P=4.305×10^4W, t=2.999×10^-4s
P=1.752×10^5W, t=5.999×10^-4s
P=3.494×10^5W, t=8.999×10^-4s
P=3.979×10^5W, t=1.2×10^-3s
P=4.431×10^5W, t=1.5×10^-3s
RFMC:
0.44 MW at t=1.5ms
p_e (W/cm^3)
ρ
P=2.782×10^5W, t=2.999×10^-4s
P=6.247×10^5W, t=5.999×10^-4s
P=8.313×10^5W, t=8.999×10^-4s
P=9.407×10^5W, t=1.2×10^-3s
P=9.763×10^5W, t=1.5×10^-3s
RFMC: 0.98 MW
at t=1.5ms
p_i (W/cm^3)
ρ
FSA p_e (W/cm^3)
p_e
P_e[W]=1.2252e+05 t[ms]=0.300
P_e[W]=2.2079e+05 t[ms]=0.600
P_e[W]=3.0751e+05 t[ms]=0.900
P_e[W]=3.8696e+05 t[ms]=1.200
P_e[W]=4.6112e+05 t[ms]=1.500
CQL3D:
0.46 MW at t=1.5ms
FSA p_i (W/cm^3)
p_i
P_i[W]=7.1154e+05 t[ms]=0.300
P_i[W]=9.8741e+05 t[ms]=0.600
P_i[W]=1.1393e+06 t[ms]=0.900
P_i[W]=1.2350e+06 t[ms]=1.200
P_i[W]=1.3002e+06 t[ms]=1.500
CQL3D:
1.3 MW at t=1.5ms

Another comparison test: NBI in NSTX, Finite-Orbit-Width (FOW)

Relaxation of Fast Ions (FI) is computed until steady-state is achieved, to t=0.1sec of phys. time (slowing down time ~60ms in plasma center).
Main challenges – need longer runs (to resolve radial transport),
Need to replenish lost particles (in ZOW, ptcls are perfectly contained within each flux surface, but not here, in FOW).

Steady state distr func ($\log_{10}$ scale) at midplane coord. R=126cm (ρ=0.3)





FI sources (from D^+-NBI) at 65keV, 32.5keV, 21.7keV

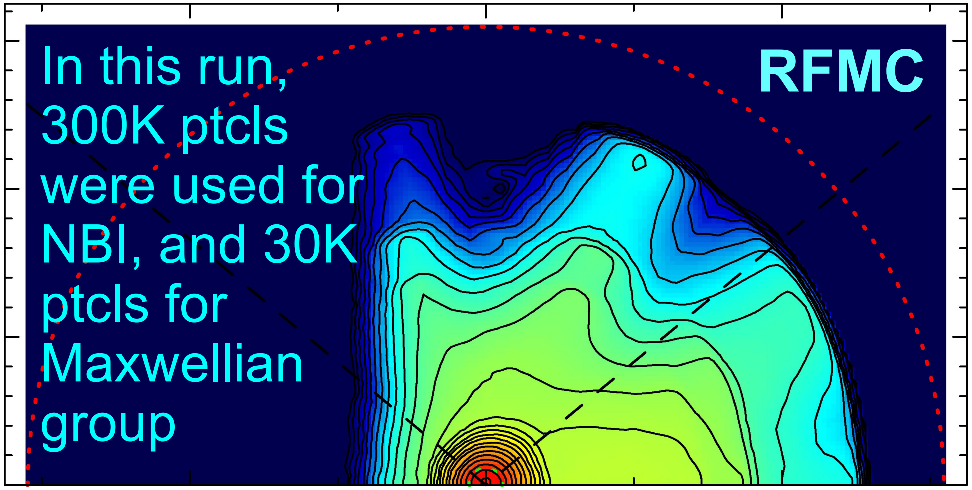
Loss "cone" (between two cyan lines)

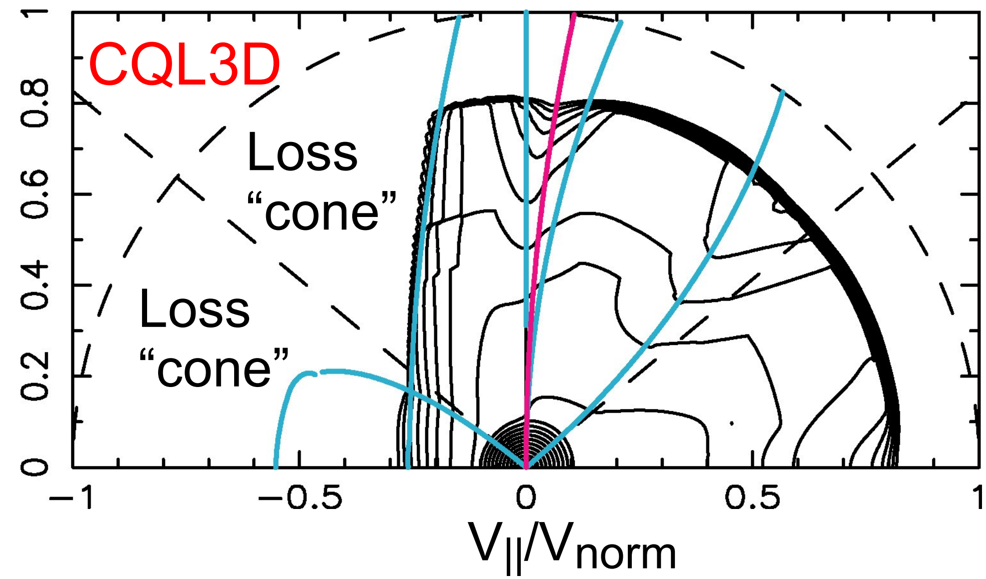
Magenta line indicates the o2 stagnation orbits

Dashed lines indicate ZOW trap-pass boundary, just for reference.
Colored lines in the CQL3D plot show FOW boundaries [ref: PPCF-58(2016)].

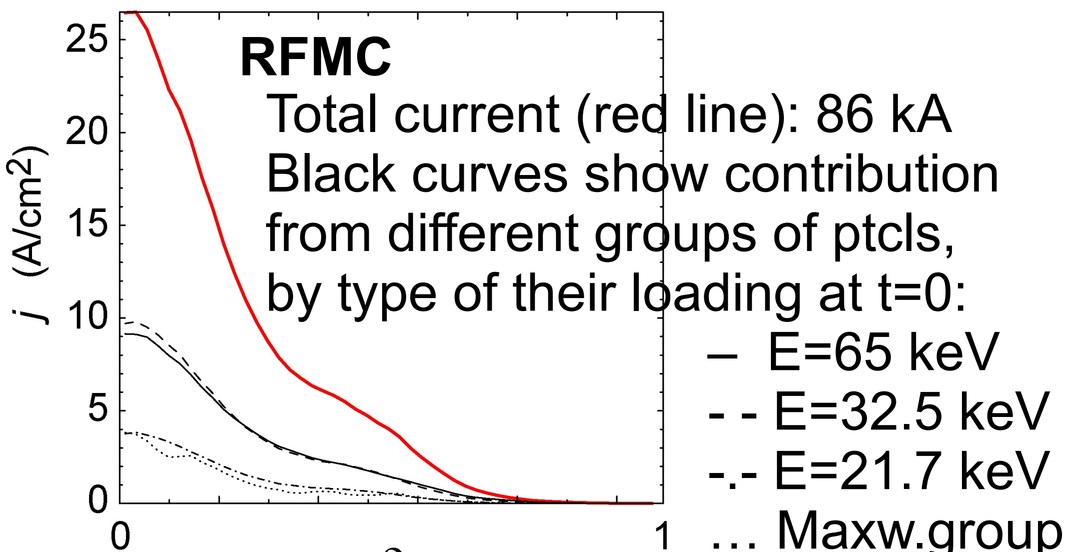
In RFMC plots, log10 levels span over 8 orders of magnitude,
in CQL3D – over 12.

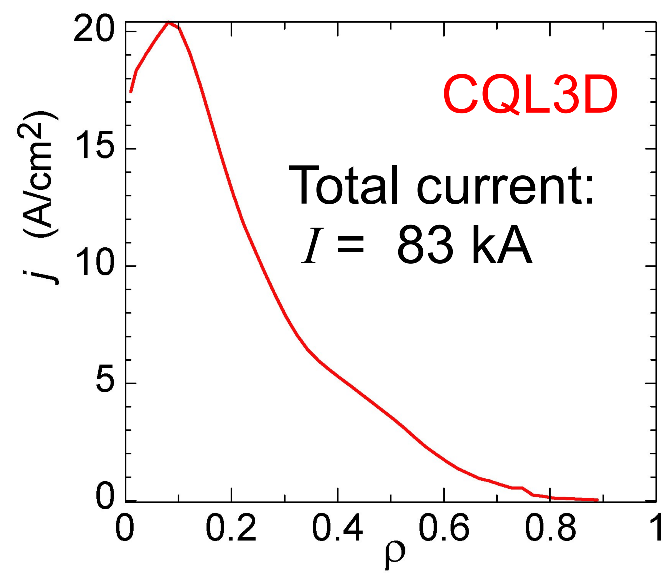
… and at midplane coord R= 140cm (ρ = 0.5)





Profiles of FSA current density



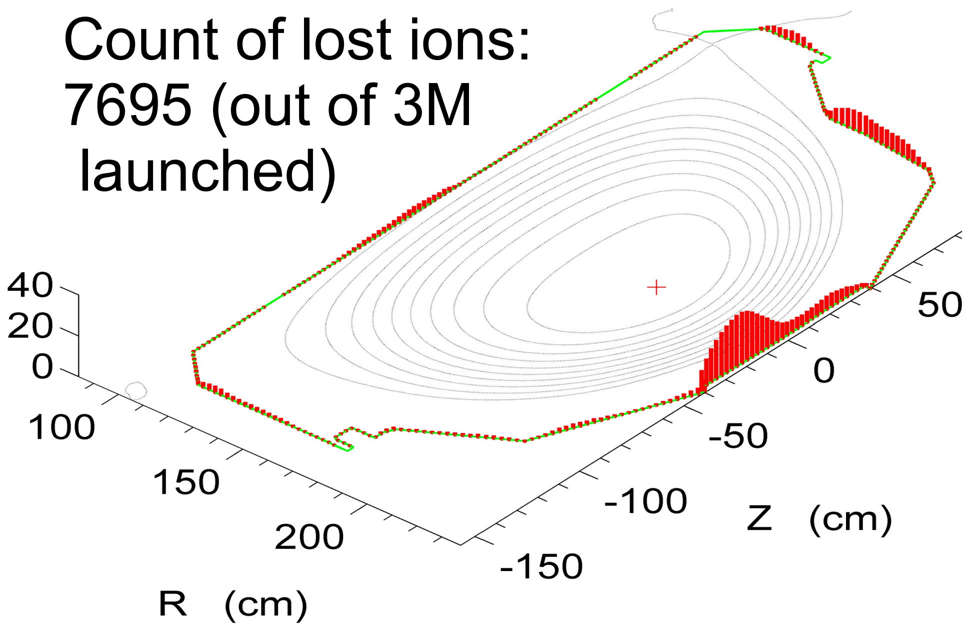


Comparing to ZOW, here in FOW the profiles of j are broader, both in RFMC and CQL3D runs.

No RF here yet – Need to import fields from TORIC (with $k_\perp$ data), or couple to GENRAY

Losses of ions and neutrals

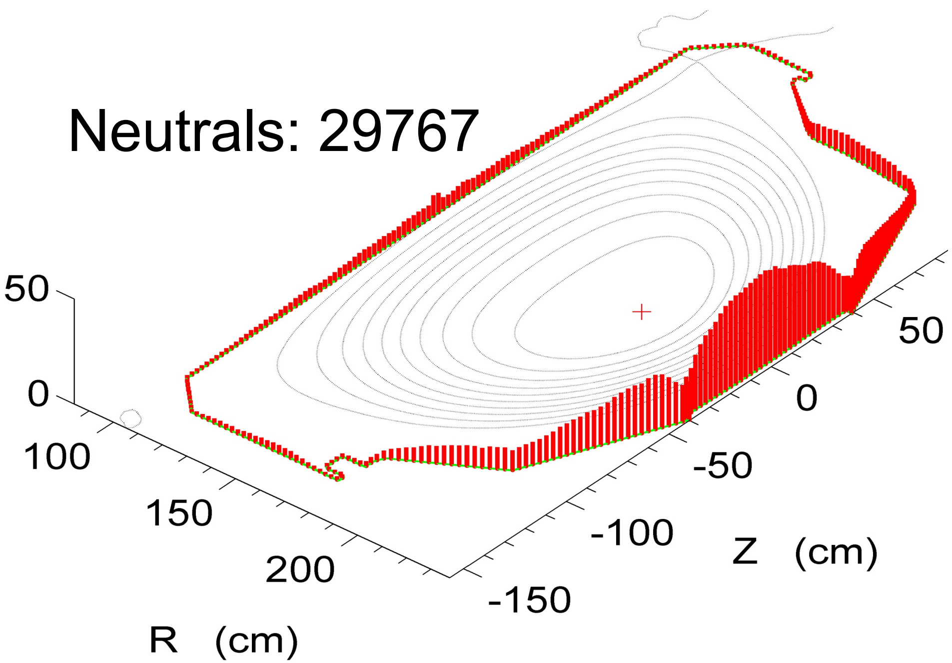
Count of lost ions: 7695 (out of 3M launched)



In this example: D^+ ions in DIII-D:

- Started as NBI-born at 70, 35 and 23.3 keV; 3M total launched ions.
- Stopped when they reach a fraction of ion thermal energy (T_i = 0.2-3.2 keV depending on r), or by **ion hitting the wall** (or by ion CX to neutral and then hitting the wall – see next plot).
  ← In this plot, prompt losses (lost in less than one bounce) are excluded.

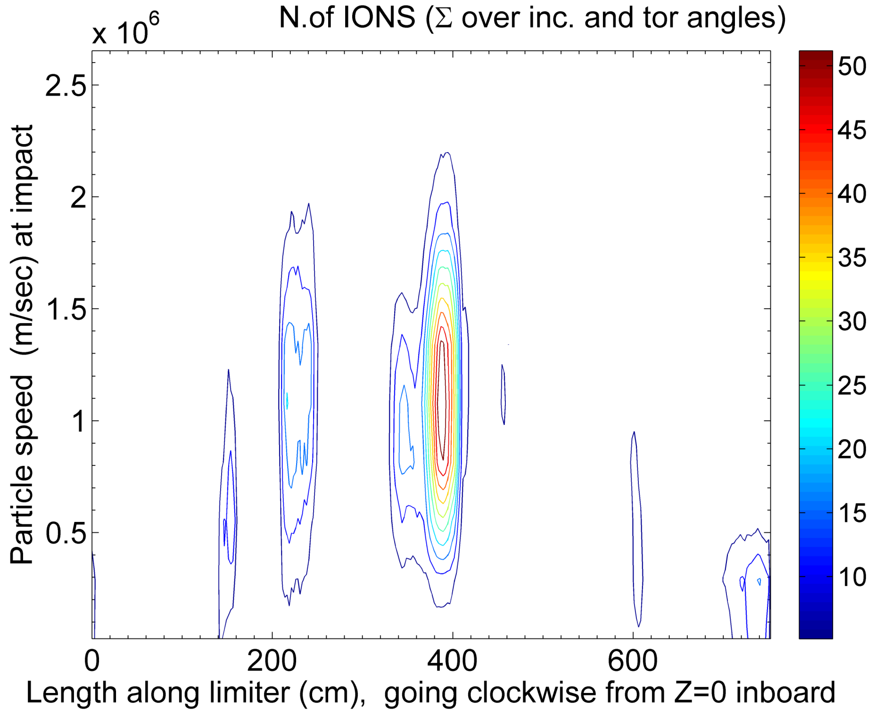
Neutrals: 29767



The count of neutrals at the wall (these neutrals are produced from CX of FI with cold neutrals) depends on neutral gas density (this run: n_n ~ 1e7-4e9 cm^{-3})

The particle is distributed among several segments of limiter according to effective “width” of trajectory => Gives smooth distributions, independent of grid.

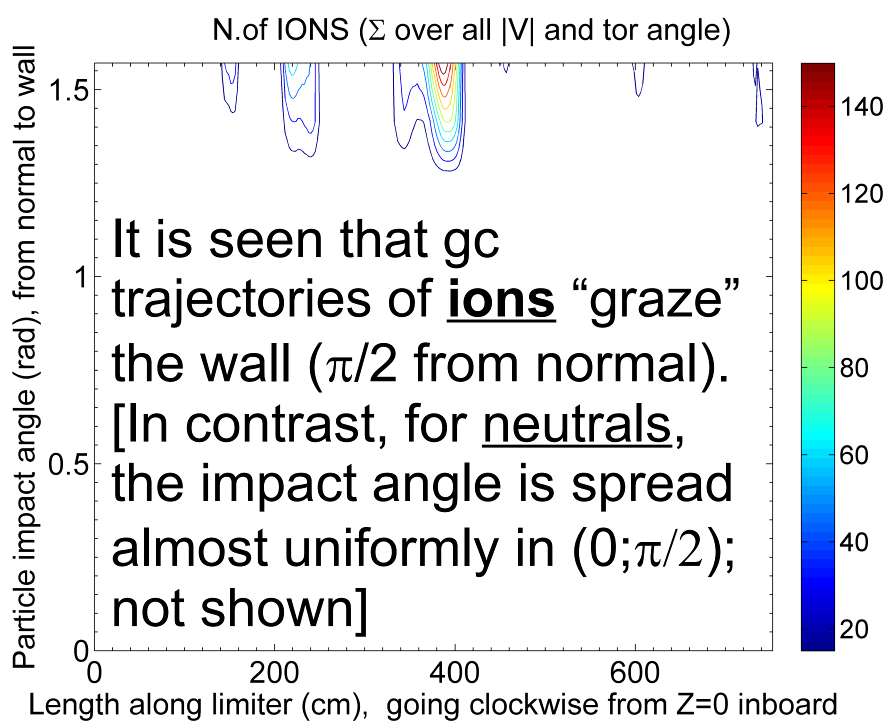
This run: 3M ptcls → tcpu=59sec on 480 cores



Lost particles are accumulated into 4D grid

- Poloidal_Length_along_limiter
- Particle_Speed_at_impact
- Incident_angle (of g.c. trajectory)
- Toroidal_angle_at_impact

← Example of plot from such data: Here, the count is summed up over all incident and tor. angles. Ions hit wall mostly at V≈1e6 m/s. [Injection speed =2.6e6 m/s (70keV) and thermal speed (0.2-0.6)e6 m/s]. Prompt ion losses (that happen in less than bounce period) are recorded separately.



It is seen that gc trajectories of **<u>ions</u>** "graze" the wall ($\pi/2$ from normal). [In contrast, for <u>neutrals</u>, the impact angle is spread almost uniformly in ($0;\pi/2$); not shown]

← Incident angle is between the vector normal to wall segment and particle gc trajectory (to be changed to full particle velocity at impact).

Future plans

- Further development of RF QL operator (Couple to GENRAY. Import QL diff. coeffs from AORSA+DC).
- Verification/comparison with CQL3D-FOW and NUBEAM, and validation against experiments.
- Improve procedure for lost ptcls – 3D details of the plasma-facing-components (PFC)/vacuum vessel, including from CAD files.
- Improve time-dependent data collection (for losses, distr.func.)
- Provide sources (particles, momentum, energy) for transport codes.
- Neutral particle model   (Degas-2, Gtneut).
- Magnetic field ripple losses.
- Add diagnostics: NPA, Coupled to FIDASIM, ...
- Explore enhanced radial diffusion due to RF and TAE activity.
- Adapt to GPU ?

APPENDIX. Plots from AORSA for C-Mod/ICRH test