The Finite-Orbit-Width (FOW) CQL3D Code Upgrade

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CQL3D Fokker-Planck System

Input:
- EQDSK equilibrium **B** field
- Time-dependent radial plasma profiles

Coupling to:
- SWIM IPS
- TRANSP
- GENRAY
- AORSA
- TORIC
- DC

CQL3D
- Bounce-Average $f_{e,i}(u_0, \theta_0, \rho, t)$
- Multi-species
- Fully 3D implicit
- Transport

Diagnostics:
- Pwr and current radial profiles
- Line-integrated Bremsstrahlung
- Neutral particle diagnostics
- Soft X-ray
- EC emission spectra
- Neutron rates
- Fusion energy reaction rates
- Bootstrap current

Storage/Visualization:
- NetCDF data files
- PGPLOT $\rightarrow$ ps files

Features:
- Toroidal DC electric field
- Large-angle e-collisions (giving knock-on elec source)
- Full nonlinear relativistic collision coeffs.
- Monte-Carlo NFREYA neutral beam source
- Loss regions in $\mathbf{u}_0$-space:
  Prompt banana losses & Ripple losses
- Radial diffusion and pinch; (u_0, θ_0, ρ)-dependence
- Up-down non-symmetrical equilibrium capability

Bounce-Average FP Equations ($\tau_B << \tau_{coll}$)

The gyro+bounce averaged FP-transport equation for the electron or ion distribution functions f_0 evaluated at the minimum magnetic field point on a flux surface:

$$\frac{\partial}{\partial t}(\lambda f_0) = \nabla_{\mathbf{u}_0}\cdot\boldsymbol{\Gamma}_{\mathbf{u}_0} + \langle\langle R(f_0)\rangle\rangle + \langle\langle S\rangle\rangle$$

$$\nabla_{\mathbf{u}_0}\cdot\boldsymbol{\Gamma}_{\mathbf{u}_0} = C(f_0) + Q(f_0) + E(f_0) + H(f_0)$$

$\langle\langle..\rangle\rangle$ is gyro/tor.angle/bounce average

C = Coulomb coll. operator
Q = rf quasilinear operator
E = Ohmic toroidal electric field
H = synchrotron radiation
R = model radial diffusion / pinch
S = particle source/sink (NBI; losses)
(C, Q, E, H conserve particles on a flux surface; R and S – do not)

– **Presently uses Zero-Orbit-Width (ZOW) approximation with COM:**
  - $\rho = \rho_0$ (Flux surface)
  - $u = u_0$ (Energy)
  - $\mu = \mu_0$ (Adiabatic invariant) $\Rightarrow$ $\sin^2\theta = [B(s)/B(s{=}0)]\sin^2\theta_0$ (where $\sin\theta = u_\perp/u$)

  The local (s) quantities on a flux surface are related to the midplane ($s{=}0$) quantities through the COM-ZOW. $f_0(\text{COM}) \equiv f_0(u_0,\theta_0,\rho) = f(u,\theta,\rho,s)$

– No coupling of u_0, θ_0 to ρ, except through phenomenological $\langle R(f_0)\rangle$.

The quantity $\lambda = |u_{||0}|\tau_B$, when multiplied by f_0, comes from the bounce-averaging process and gives the number of particles per unit cross-section area of a flux tube, and per $d^3\mathbf{u}_0$.

FOW modification replaces simple ZOW orbits with full guiding center orbits:
$\Rightarrow$ (Large orbit) Neoclassical rad transport, accurate losses, accurate distn f.

FOW modifications: Main computational challenge – collision operator

$$\left(\frac{\partial f_a(\mathbf{u})}{\partial t}\right)_C \equiv C_{ab}(f_a, f_b) = \frac{\partial}{\partial \mathbf{u}}\cdot\left[\mathbf{D}_{ab}\cdot\frac{\partial f_a(\mathbf{u})}{\partial \mathbf{u}} - \mathbf{F}_{ab} f_a(\mathbf{u})\right]$$

where $\mathbf{u}$ is the momentum per rest mass, and $\mathbf{D}_{ab}$ and $\mathbf{F}_{ab}$ are the diffusion and friction coefficients; a,b=(elec,ions),

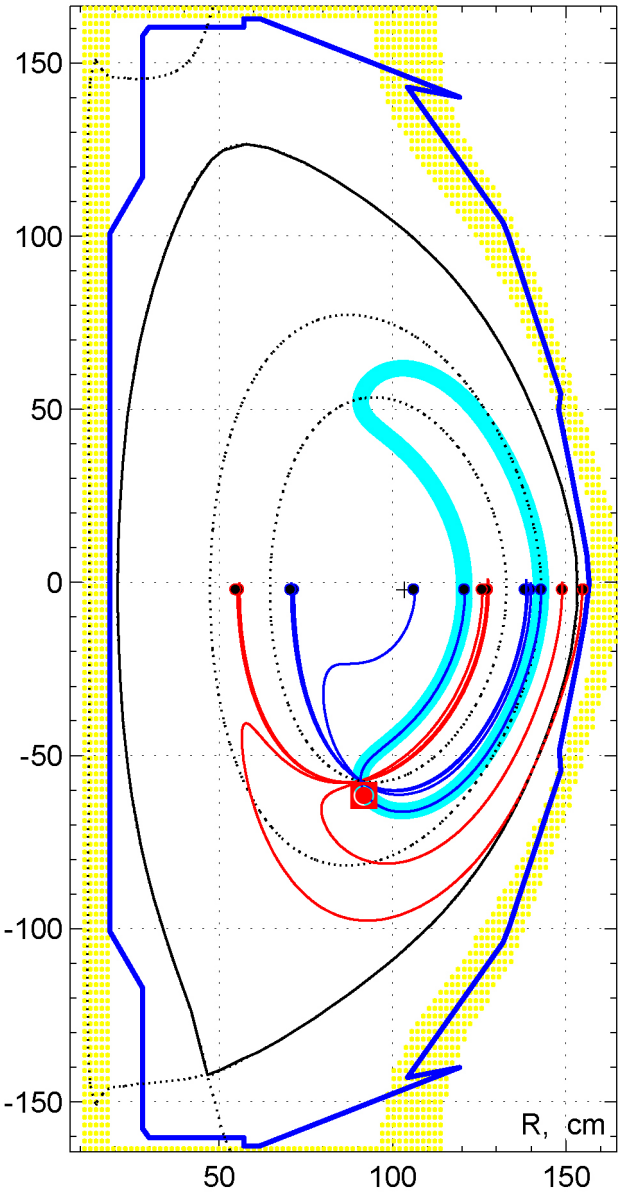
$$\mathbf{D}_{ab}(\mathbf{u}) = \tfrac{1}{2}\,\Gamma_a \sum_b (Z_b/Z_a)^2 \ln\Lambda_{ab} \int \mathbf{U}(\mathbf{u},\mathbf{u}') f_b(\mathbf{u}') d^3\mathbf{u}'$$

$$\mathbf{F}_{ab}(\mathbf{u}) = -\tfrac{1}{2}\,\Gamma_a \sum_b (Z_b/Z_a)^2 (m_a/m_b) \ln\Lambda_{ab} \int (\nabla_{\mathbf{u}'}\cdot\mathbf{U}(\mathbf{u},\mathbf{u}')) f_b(\mathbf{u}') d^3\mathbf{u}'$$

- This is the *local* form of the collisional operator, which involves *local* distributions of "main" (f_a) and "secondary" (f_b) species, at each pt on orbit.
- However, in the bounce-average formulation of the Fokker-Plank equation, the distribution function is only known as a function of three Constants of Motion (COM).
- For convenience, we choose the COM to be (R_0, u_0, θ_0) that specify the radial bin on the midplane where the bounce-average distribution is calculated, and the particle momentum and pitch angle at this point.
- This "convenient COM" can be easily linked to the COM triplet (u^2, μ, p_φ) of energy, magnetic moment and canonical toroidal momentum.

Bounce-averaging procedure in the FOW case:

1. For each R_0-bin, "main" orbits are launched on (u_0, θ_0)-grid.
2. For each "main" orbit, a set of points is selected on the orbit to be used for bounce-averaging of the collisional operator.
3. From each selected point, the "secondary" orbits are launched on (u', θ')-grid, and traced to the midplane, thus determining the local f_b of the "secondary" species from the midplane f_{b0}.



Plot: "Main" orbit (**bold**) – 29 keV deuteron in NSTX, θ =0.65 rad; "Secondary" orbits (thin lines), 29 keV, $\theta' = 0 - \pi$, are launched from one selected point (◙) and stopped at the equatorial plane.

The integration in $\mathbf{D}_{ab}$ and $\mathbf{F}_{ab}$ is performed over "secondary" orbits. After this procedure is repeated for all selected points on main orbit, the bounce-average collisional operator is found.

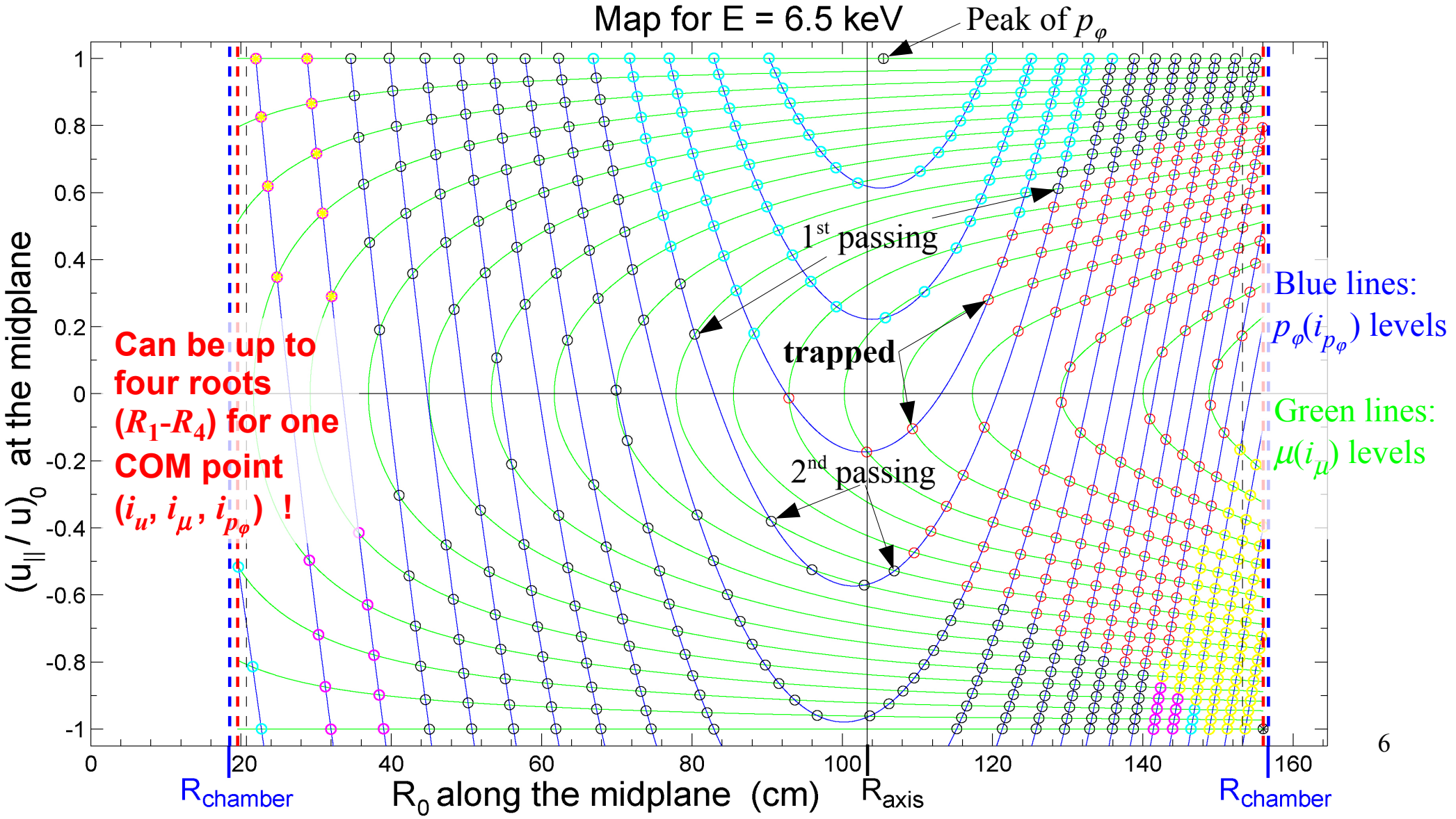
Direct orbit tracing – too "pricy" CPU time: 4 flux-surfaces $\times$ 40 vel. $\times$ 60 pitch angles to launch "main" orbits $\times$ 20 points selected on each "main" orbit $\times$ 40 vel. $\times$ 60 pitch angles for "secondary" orbits = 460,800,000 orbits $\rightarrow$ 270 min.

Alternative, CPU-time efficient approach: Make a look-up table for $R_{midplane}$ that depends on three indices corresponding to COM = $(u,\ \mu,\ p_\varphi)$ [μ and p_φ defined over equispaced grids $p_\varphi(i_{p_\varphi})$, $\mu(i_\mu)$]. Use this table for a fast determination of equatorial R_0' for the "secondary" orbits: At each point (R, Z) on the "main" orbit, and each given (u', θ') for the "secondary" orbit, find (u', μ', p_φ') constants and look up for (R_0', θ_0') in the table.

Construction of the Look-up Table COM → $R_{midplane}$, $\theta_{midplane}$

For a given u, plot the levels of $p_\varphi = (Ze/mc)\Psi_{pol} + (B_\varphi/B)R_0 u_0 \cos\theta_0$ and the levels of $\mu = (1-\cos^2\theta_0)/B$ (normalized adiab. invariant) as a function of $R_0 \equiv R_{midplane}$ and $\cos\theta_0 = (u_{||}/u)_0$, and find all intersections. Done for the grid of $p_\varphi(i_{p_\varphi})$, $\mu(i_\mu)$ values.

Similar to [J. Egedal, Nucl.Fus. **40**, 1597 (2000)], but here all intersection points are found numerically:



Map COM → $R_{midplane}$, $\theta_{midplane}$ for 6.5 keV

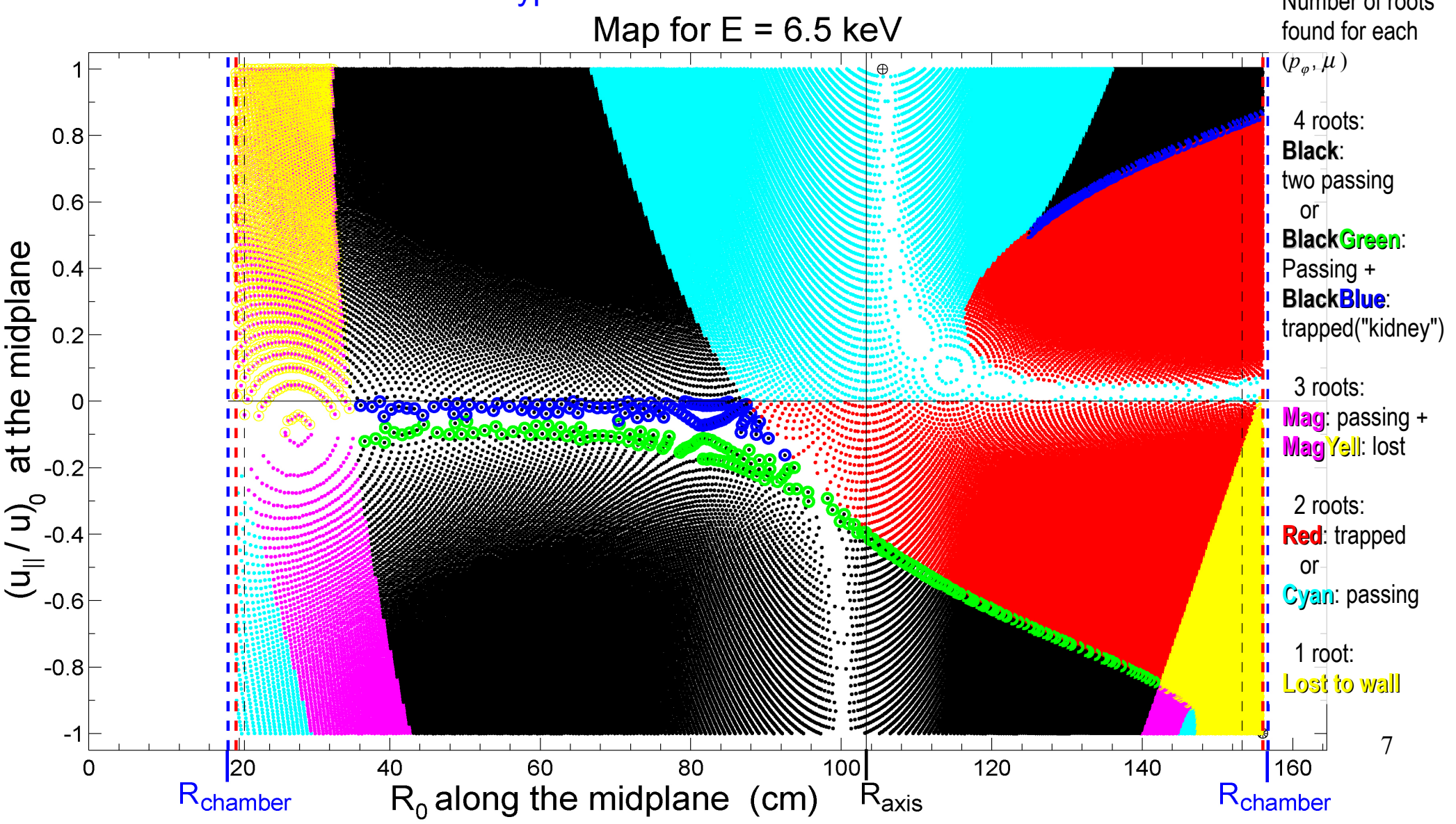
The total (80 energy levels) table size is (N_u, N_μ, N_{p_φ}) = 80×300×300×(4 roots).

Total CPU time = ~100 sec.; calculated once, before time loop starts.

Here, a map is shown for one energy level, with 300×300 intersecting levels in μ and p_φ .

Levels are not shown, only the intersection points.

Colors indicate different orbit types / number of roots.



The look-up table is used for a fast search of $R_{midplane}$ for the secondary orbits – shown with dots in the figure, compared to orbits:

The test run with 460,800,000 orbits (4 flux-surfaces, 40×60 main orbits, 20 selected points on each main orbit, 40×60 secondary orbits) took 1 min (vs. 270 min for orbits).

For refined grid with 32 flux-surfaces, 80 pts per orbit, and $(80\times80)^2$ velocity-space, projected CPU time will be ~4 hours (but can speed up by ~100 with inexpensive multi-core Graphics Processing Unit).

The next step in the FOW modification is to calculate the nonlinear ion collision operator, as a generalization of present zero-orbit-width methods in CQL3D.

The target application is analysis of FOW effects in NSTX, giving accurate neocl. transport, accurate orbit losses (incl spectra), accurate ion diagnostics (FIDA, NPA), and accurate ion distributions with NBI and full wave AORSA. **All are strongly affected by FOW.**