Scientific Progress in the Center for Simulation of Wave-Plasma Interactions

SciDAC Advisory Committee Meeting

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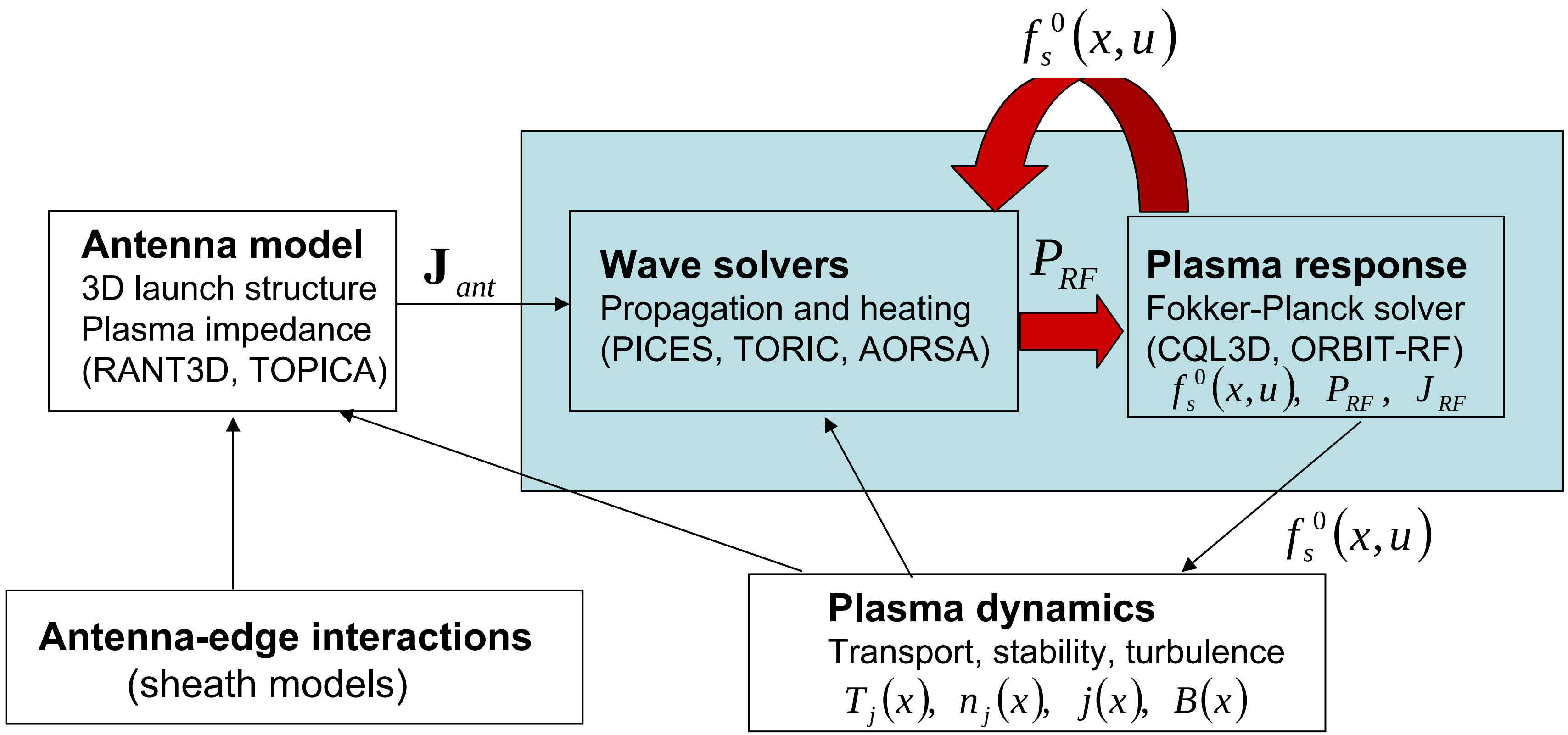
Review Progress in Four Key Areas

- Quasilinear evolution of nonthermal ion distributions:
  - Fast Wave – beam interaction in DIII-D
  - Energetic ion tail formation in minority ICRH in Alcator C-Mod
  - Identification of importance of finite ion orbit effects
  - Assessment of validity of quasilinear theory
- Application of ICRF full-wave solvers to ITER:
  - Simulation of mode conversion scenario and code benchmarking activity
- Self-consistent simulations of LHCD:
  - Coupled Fokker Planck – full-wave solver
- Simulations of driven particle modes using full-wave solver.
- Simulations of edge plasma – ICRF antenna interaction:
  - Linear coupling with 3D antenna code and full-wave solver.
  - Nonlinear formation of RF sheaths

- **Progress in each area will be described in terms of physics understanding, algorithms and computer science, and future directions**

Iteration Scheme for Physics Packages



Wave propagation and the plasma response are governed by the Maxwell-Boltzmann system of equations

For time harmonic (rapidly oscillating) wave fields **E** with frequency ω, Maxwell's equations reduce to the Helmholtz wave equation

$$-\nabla\times\nabla\times\mathbf{E}+\frac{\omega^2}{c^2}\left(\mathbf{E}+\frac{i}{\omega\varepsilon_0}\mathbf{J}_p\right)=-i\omega\mu_0\mathbf{J}_{ant}$$

The plasma current ($\mathbf{J}_p$) is a non-local, integral operator (and non-linear) on the rf electric field and conductivity kernel;

$$\mathbf{J}_p(\mathbf{r},t)=\sum_s\int d\mathbf{r}'\int_{-\infty}^{t}dt'\sigma\left(f_{0,s}(E),\mathbf{r},\mathbf{r}',t,t'\right)\cdot\mathbf{E}(\mathbf{r}',t')$$

Wave Solver (AORSA)

The long time scale response of the plasma distribution function is obtained from the bounce averaged Fokker-Planck equation

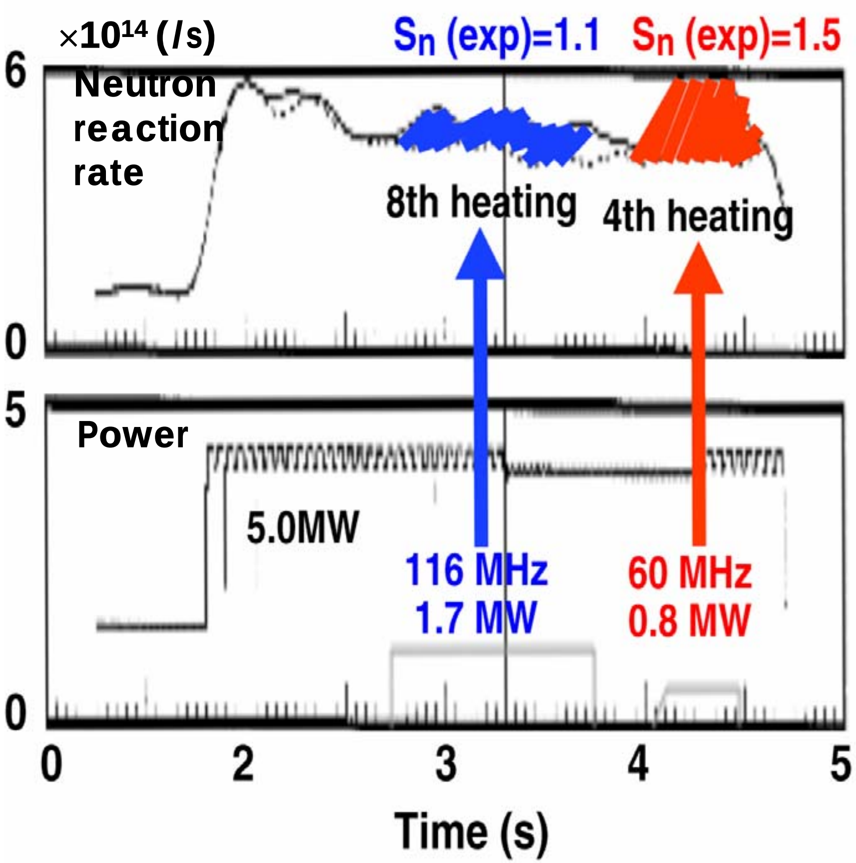
$$\frac{\partial}{\partial t}(\lambda f_0)=\nabla_{\mathbf{u}_0}\cdot\Gamma_{\mathbf{u}_0}+\langle\langle S\rangle\rangle+\cancelto{0}{\langle\langle R\rangle\rangle}\quad \text{where}\quad \nabla_{\mathbf{u}}\cdot\Gamma_{\mathbf{u}}=C(f_0)+Q(\mathbf{E},f_0)$$

Plasma Response (CQL3D)

Need to solve this nonlinear, integral set of equations for wave fields and velocity distribution function self-consistently. This requires an iterative process to attain self-consistency.

Puzzle arose from initial simulations of high harmonic fast wave (HHFW) – fast ion beam interaction in DIII-D

- DIII–D high density L-mode



S_n: neutron enhancement factor

Stronger Beam Interactions at $4\Omega_D$ (60 MHz) Than at $8\Omega_D$ (116 MHz) Observed in DIII-D

CQL3D-AORSA predicted increased absorption as frequency was raised.

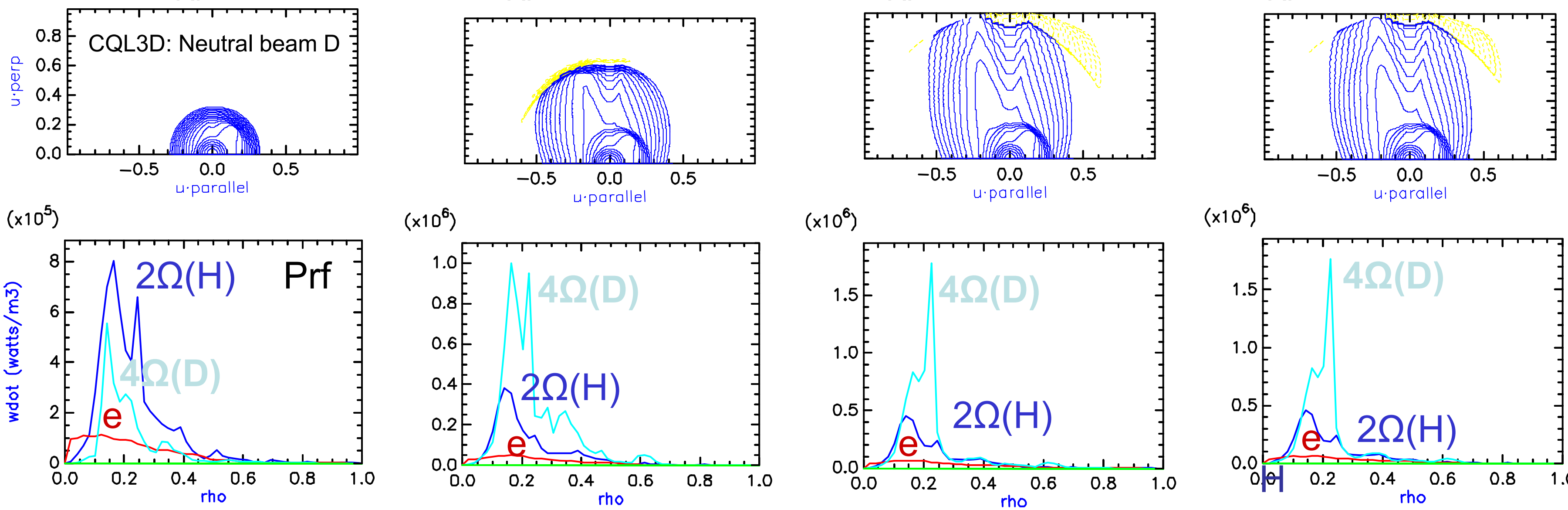
Monte Carlo ORBIT code (ORBIT-RF) combined with an RF operator (using fields from TORIC solver) did reproduce the experimental trend.

Could finite ion orbit effects be playing a role ?

AORSA and CQL3D were iterated to solve for the wave fields and distribution function self-consistently in the DIII-D HHFW – NBI Interaction

f = 60 MHz (4th harmonic D; non-Maxwellian) and 2% minority H (2^{nd} harmonic H, Maxwellian)

0^{th} iteration	1^{st} iteration	5^{th} iteration	6^{th} iteration
$P_{RF} = 0$	P_{RF} = 1.1 MW	P_{RF} = 1.1 MW	P_{RF} = 1.1 MW



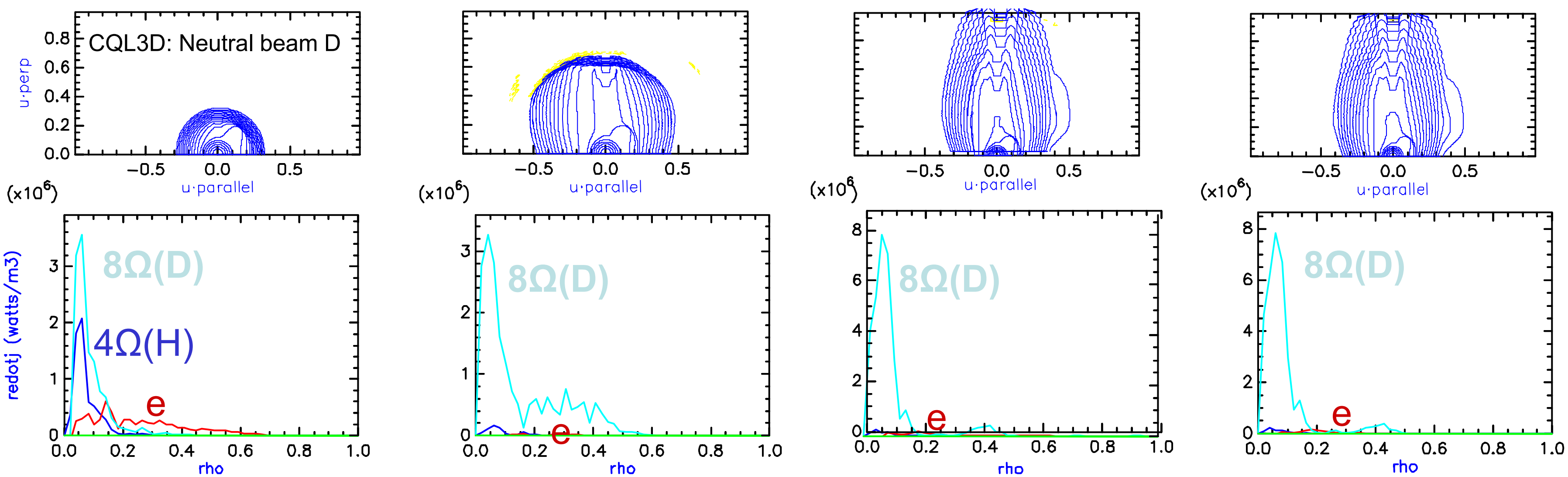
P(D) = 0.29 MW = 23.8 %	P(D) = 0.84MW = 66.3 %	P(D) = 0.76 MW = 58.2 %	P(D) = 0.75 MW = 57.1%

At 60 MHz, about 57% of the RF power is absorbed by the deuterium

At 116 MHz, about 95% of the power is absorbed by the deuterium beam

f = 116 MHz (8th harmonic D; non-Maxwellian) and 2% minority H (4th harmonic H, Maxwellian)

0th iteration	1st iteration	7th iteration	8th iteration
$P_{RF} = 0$	$P_{RF} = 1.6$ MW	$P_{RF} = 1.6$ MW	$P_{RF} = 1.6$ MW



0th iteration	1st iteration	7th iteration	8th iteration
P(D) = .55 MW = 34.5 %	P(D) = 1.54MW = 96.2 %	P(D) = 1.47 MW = 92.3 %	P(D) = 1.50 MW = 94.6 %

This is in disagreement with the experiment which shows little power absorbed at the 8th harmonic (One possible explanation is that radial diffusion and finite orbit effects are becoming important at the higher frequency).

Finite orbit effects have been studied quantitatively using a Monte Carlo Approach: ORBIT RF Code coupled with an RF Operator - [Choi & Chan, 2005]

QL Diffusion Operator Formulated in terms of Multi-Fourier Poloidal Modes from the TORIC ICRF Solver and used to compute increment in magnetic moment due to the ICRF interaction:

$$\Delta\mu_{rf} = \overline{\Delta\mu_{rf}} + R_s\sqrt{\left\langle \overline{\overline{\Delta\mu_{rf}}}^{2} \right\rangle}$$

$$D_n(k_{//}) = \frac{\pi B\mu}{m_i} K\delta(\omega_n)\sum_{k'} D^{*}_{\perp n}(k')\sum_{k} D_{\perp n}(k)$$

$$\overline{\Delta\mu_{rf}} = \int_{\Delta t} dt\,\frac{q^2 n^2 \Omega^2}{\omega^2 B^2}\frac{\partial D_n(k_{//})}{\partial\mu}$$

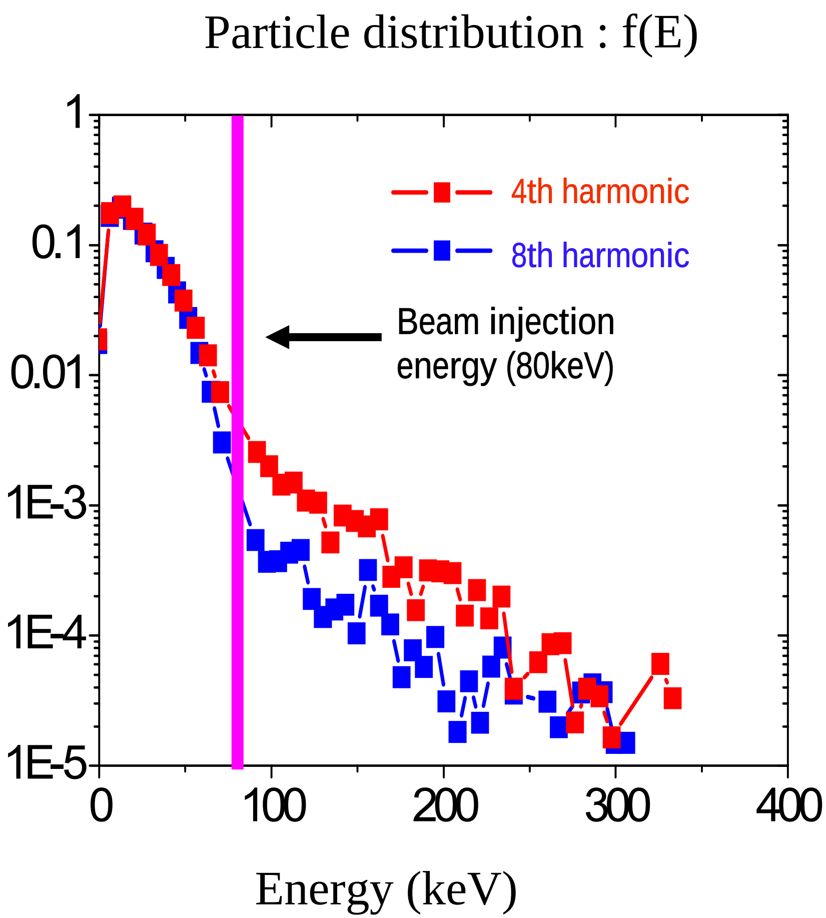
$$\omega_n = \omega - l\Omega - k_{//}\mathrm{v}_{//}$$

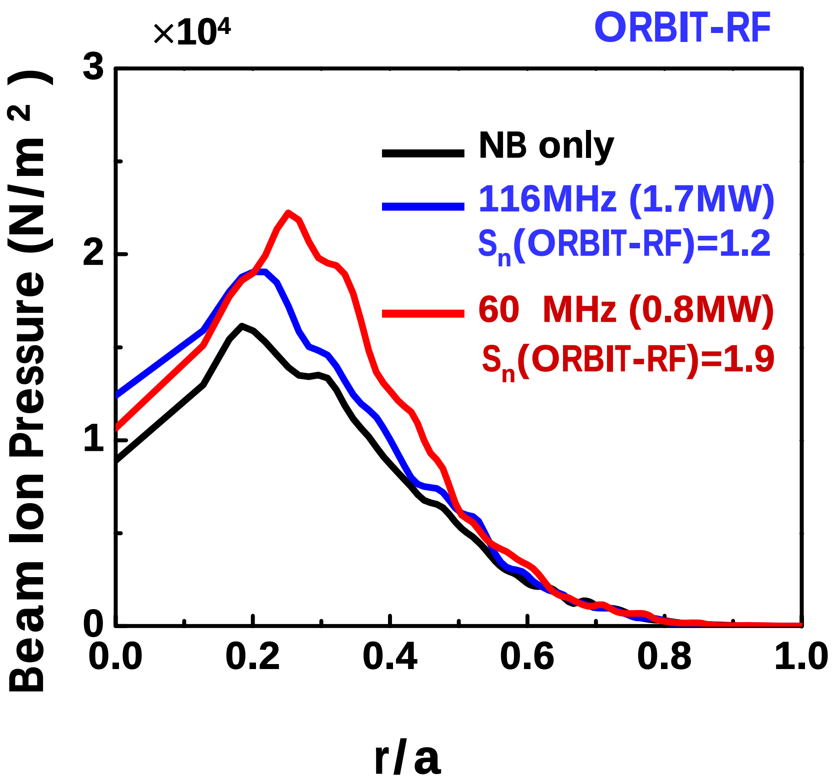
$$\left\langle \overline{\overline{\Delta\mu_{rf}}}^{2} \right\rangle = \int_{\Delta t} dt\,\frac{2q^2 n^2 \Omega^2}{\omega^2 B^2} D_n(k_{//})$$

$$\sum_{k} D_{\perp n}(k) = \sum_{m} E_{+}^{m} J_{n-1}(k_{\perp}^{m}\rho_i)$$

Collision operator includes Coulomb collisions with plasma ions and electrons and change in pitch angle due to scattering of test ions from background ions.

Beam pressure computed with *f*(E) from ORBIT-RF agrees qualitatively with experiment – but why ?





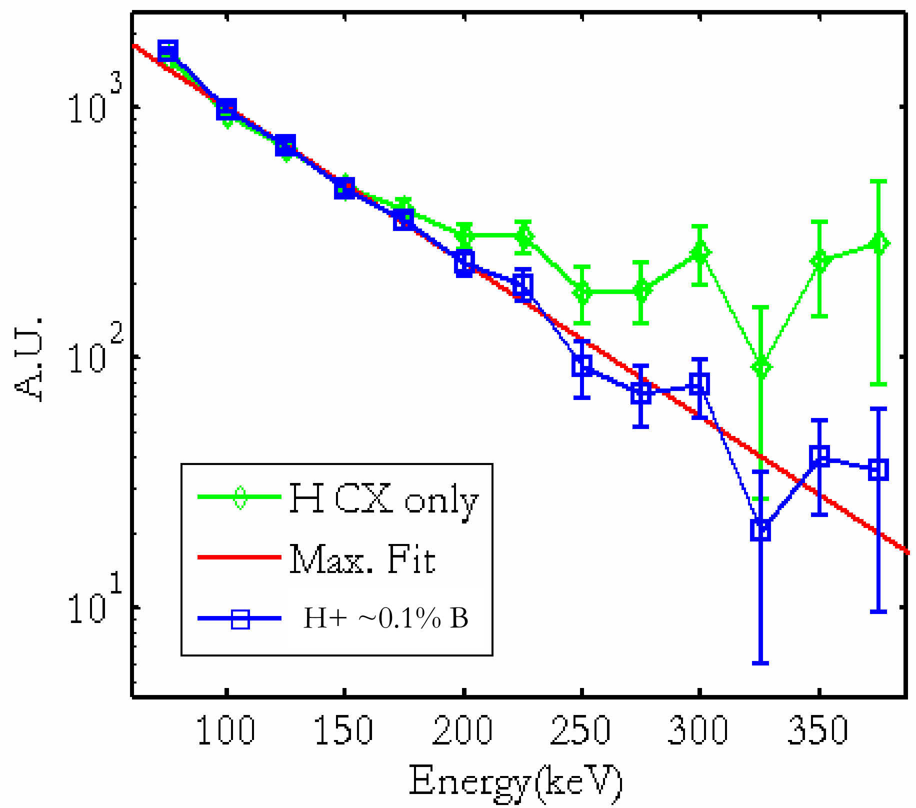
Decided to compare AORSA/CQL3D and ORBIT-RF on a minority ion heating case from Alcator C-Mod

Fundamental minority ion absorption is well-understood.

Relatively low energetic tail energies might render finite ion orbit effects less important.

Good experimental measurements of the energetic ion tail have been made using a compact neutral particle analyzer (CNPA)

- **Using a Maxwellian fit to data gives $T_{ion} \sim 70$ keV.**



Courtesy of Vincent Tang, MIT (APS, 2005)

AORSA and CQL3D have now been coupled iteratively on the same computing platform

- The Python iteration is a stand-alone system in which both codes communicate and interact automatically on the same computing platform (Cray XT-3 at ORNL)
- The combined simulation has restart capability after each iteration.
- The combined, self-consistent model was used to simulate the quasilinear evolution of the minority hydrogen (H) distribution function during ICRF heating experiments in the Alcator C-Mod tokamak.
- This advance benefited greatly from CS expertise at ORNL.

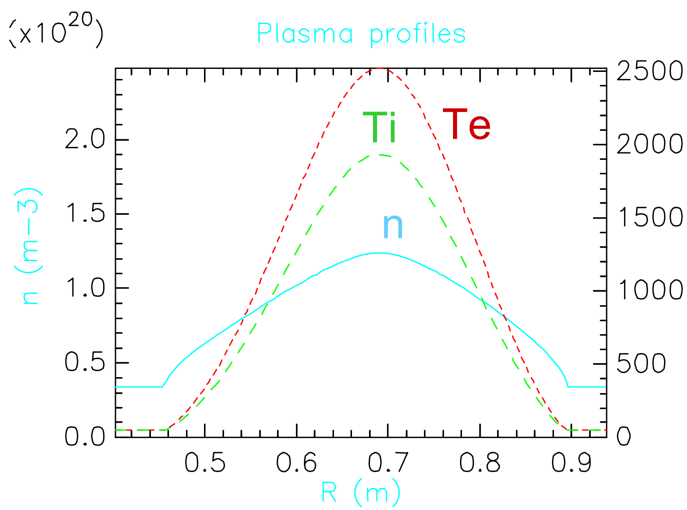
C-Mod Minority H Benchmark Case

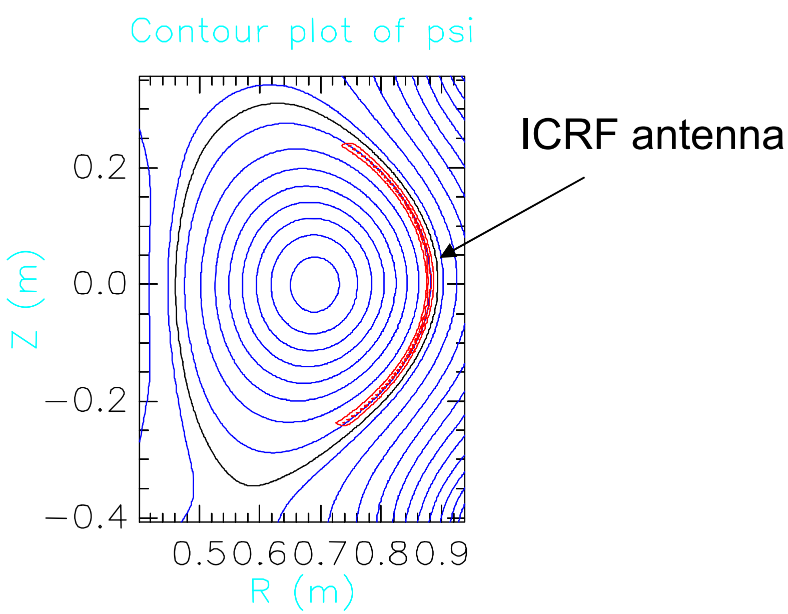
Plasma parameters:

Shot #1051206002.01120
$n_e(0) = 1.277 \times 10^{20}\ m^{-3}$
$T_e(0) = 2.609$ keV
$T_i(0) = 2.00$ keV
$n_H / n_e = 8\%$
n_D from quasi-neutrality
$B_0 = 5.41$ T

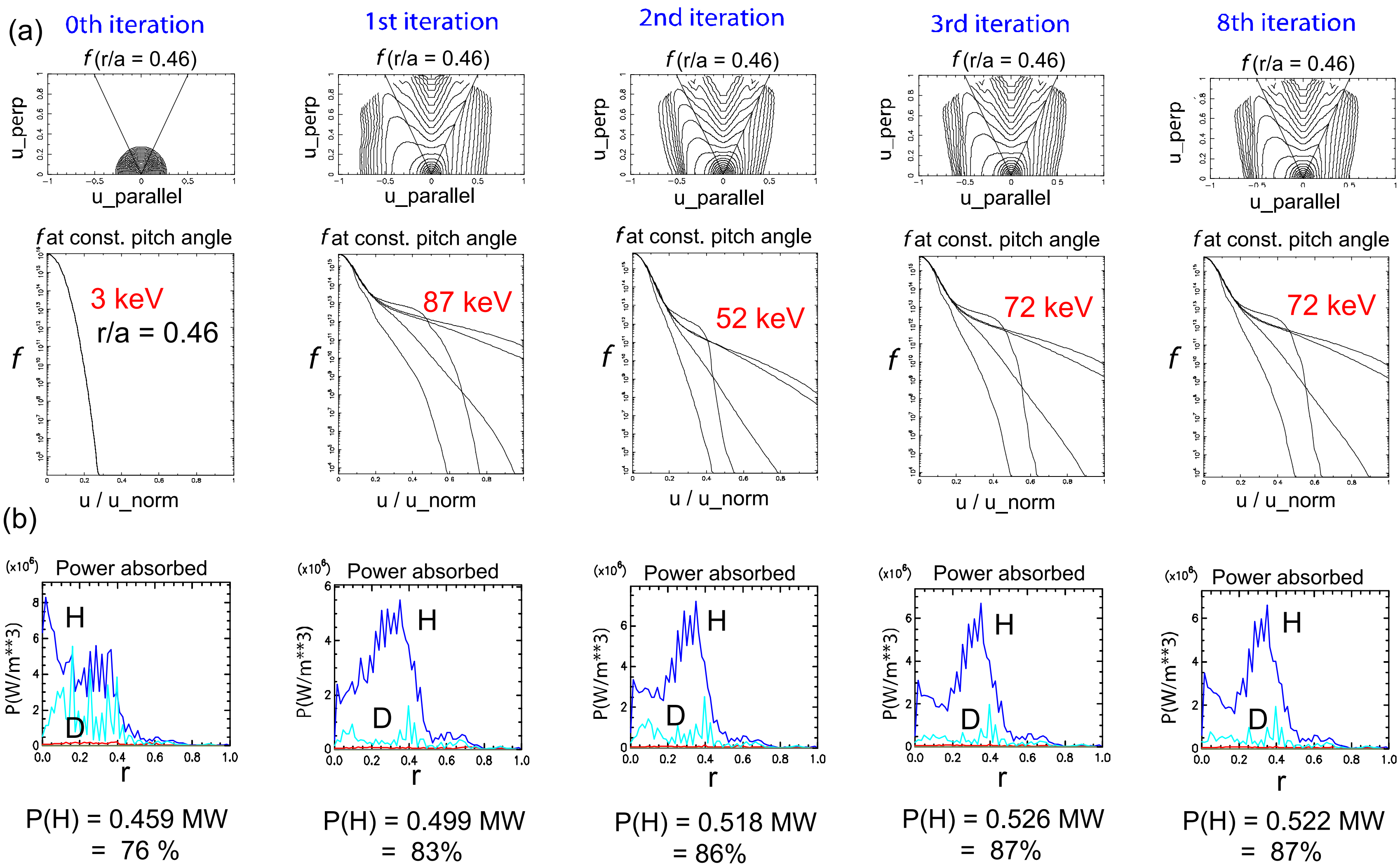
ICRF Parameters:

$f = 80$ MHz
$n_\varphi = 10$
$P_{rf} = 600$ kW
$H_{ant} = 0.48$ m
$R_{ant} = 0.88$ m
$J_{ant}(y) = J_0 \cos(k_y\ y)$
$k_y = \omega/v_{ph}$ *where* $c/v_{ph} = 1.6$

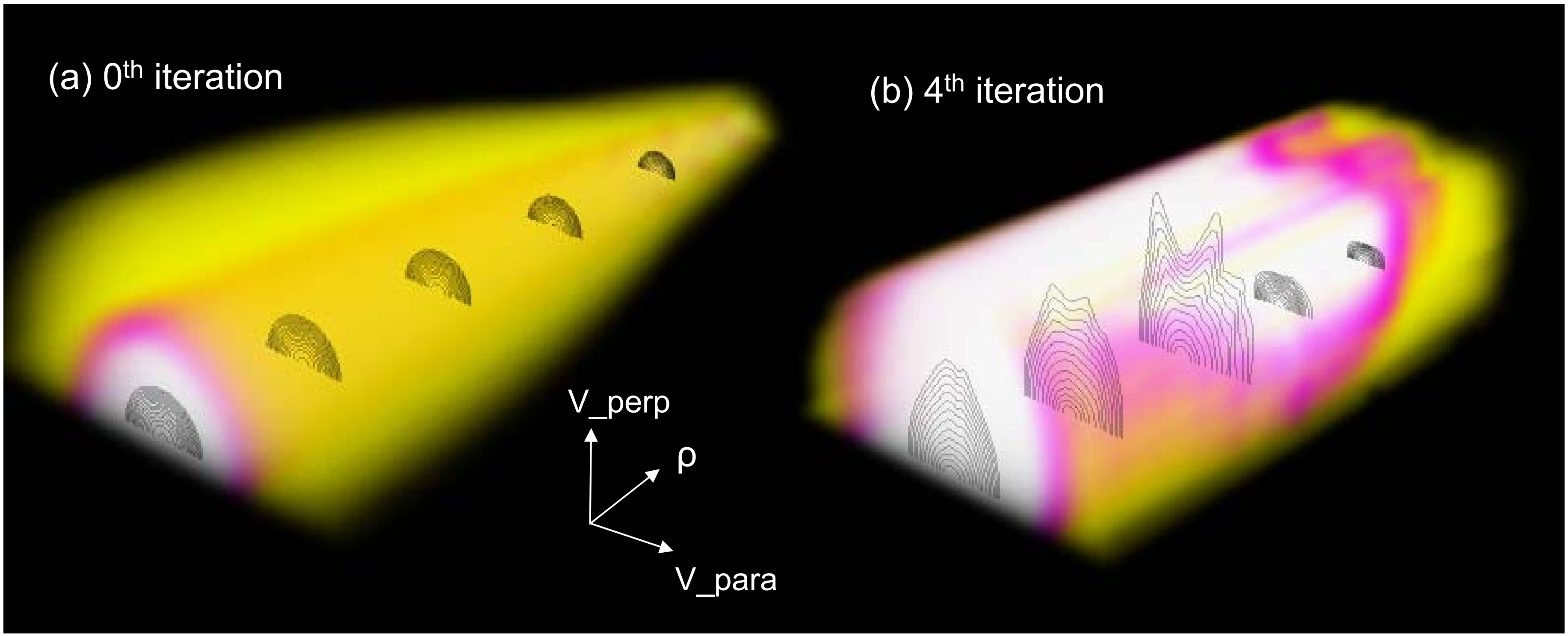




Iteration for C-Mod minority H, N_R = 128, N_Z = 128, [256 processors for 3 hrs on Cray XT3 – ORNL]

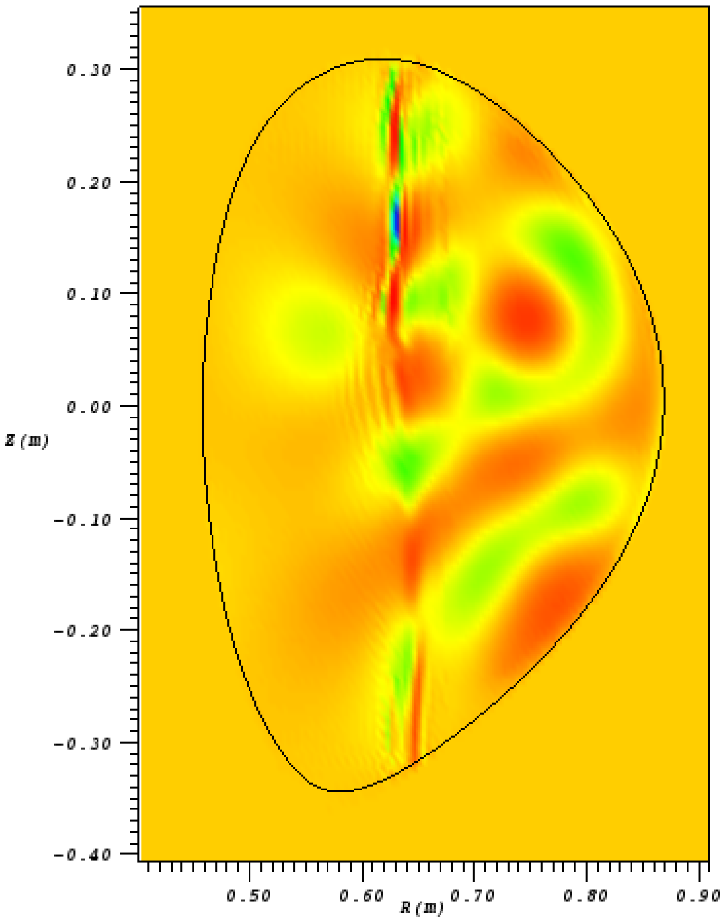


Bounce-averaged distribution function for H minority in Alcator C-Mod, N_R = 128, N_Z = 128

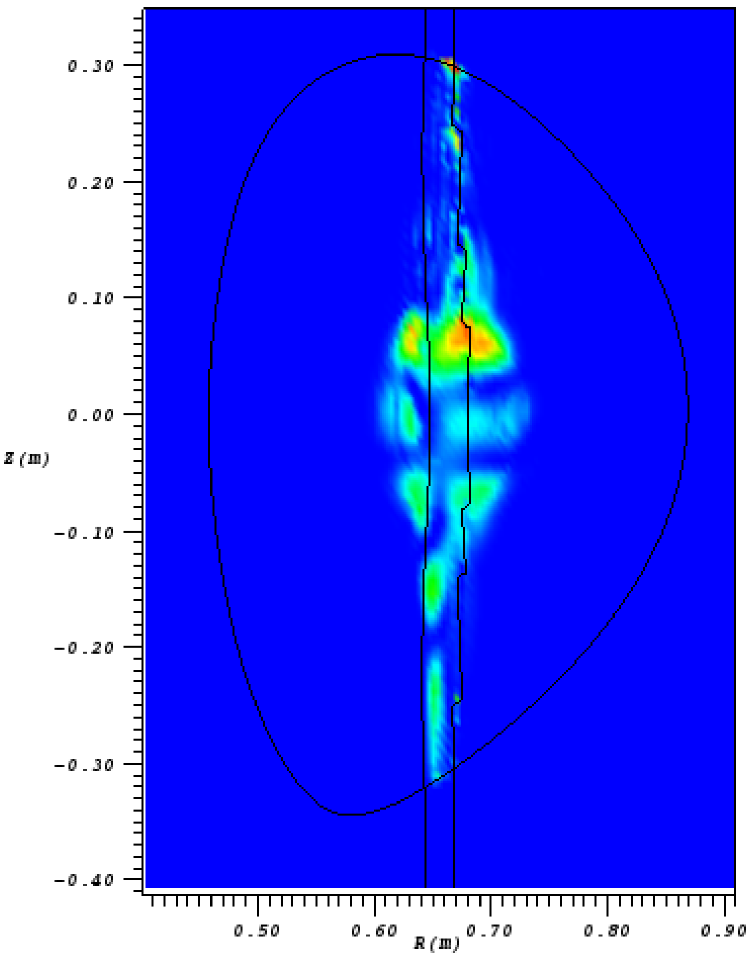


Wave fields and minority heating for the converged solution N_R = 128, N_Z = 128

Wave fields

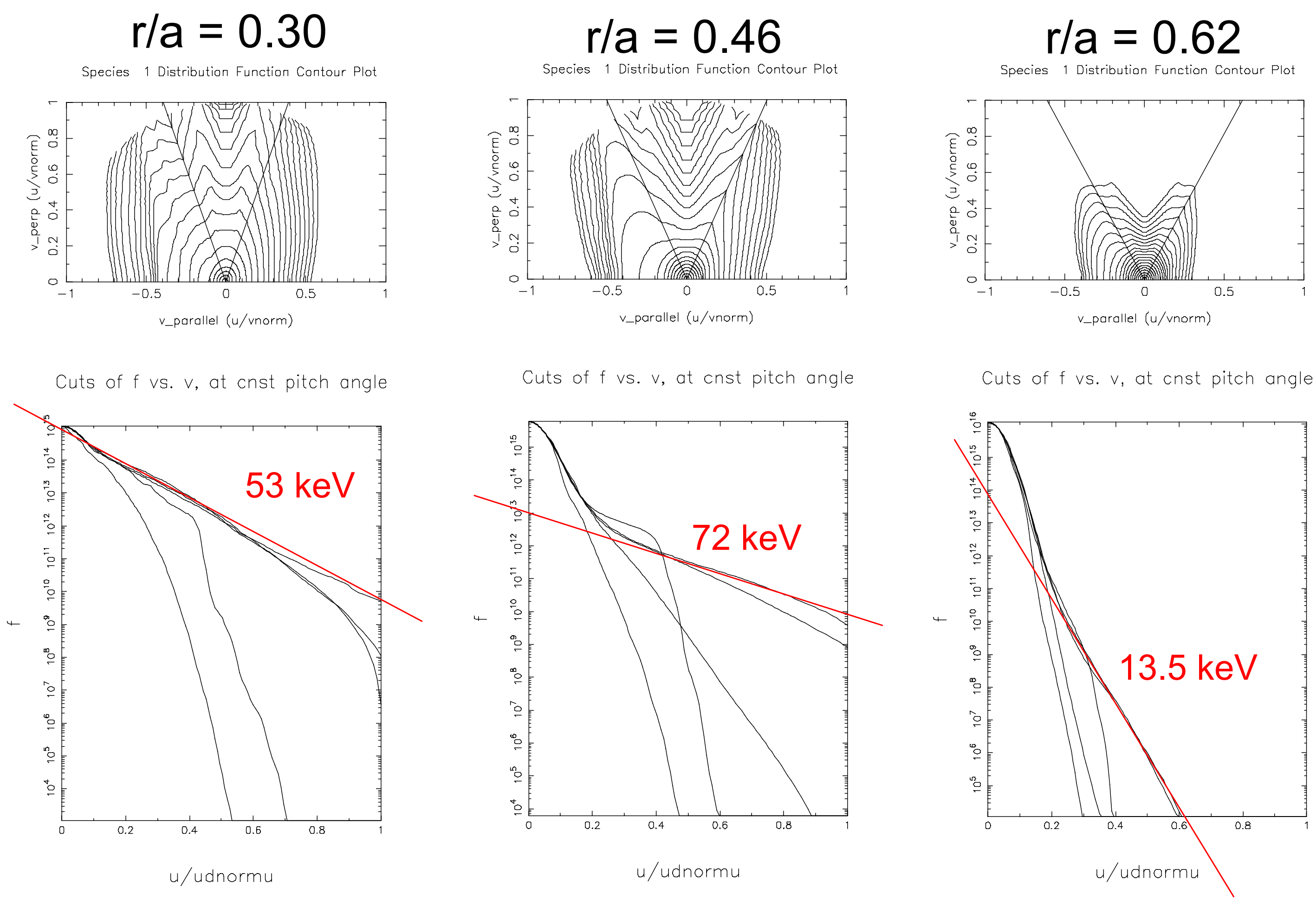


Heating (H)



Tail temperature peaks at about r/a = 0.46 where heating is maximum N_R = 128, N_Z = 128

Predicted tail temperature (72 keV) agrees closely with experimental measurement (70 keV)



The diffusion coefficient (D) has also been evaluated by a direct orbit integration using electric fields from AORSA

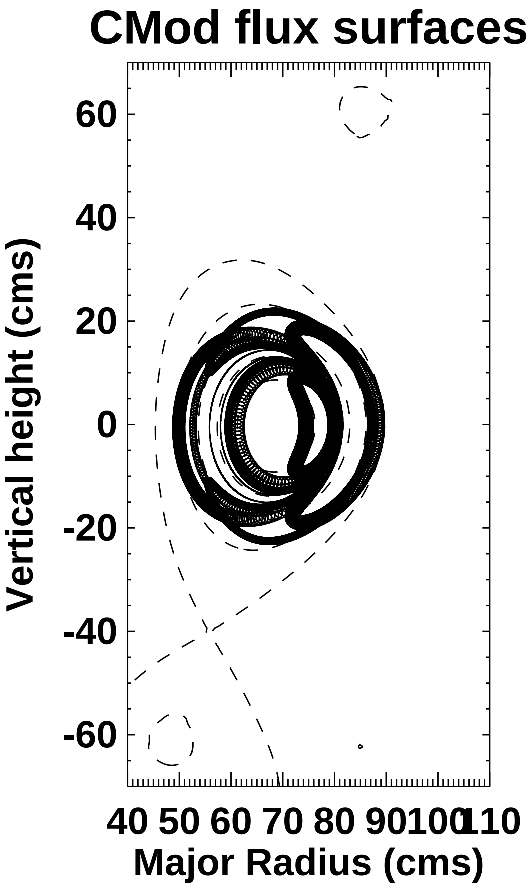
- "DC" calculates the bounce average rf (not quasilinear) diffusion coefficients as a function of ($v_{//}$, $v_{\perp}$, r):
  - Particles are followed for one (or more) complete poloidal transits by numerically integrating the Lorentz force equation.
  - A suite of orbits with initial conditions chosen to provide a gyro- and toroidal-average for each ($v_{//}$, $v_{\perp}$, r) constants-of- motion (COM) point.
  - Method is statictical and therefore avoids noise.

- Magnitudes and general radial profiles of D from Lorentz Orbit Code (DC) and bounce averaged calculation – AORSA/CQL3D are similar.

- However, significant differences also exist in D that are most likely due to finite orbit width effects.

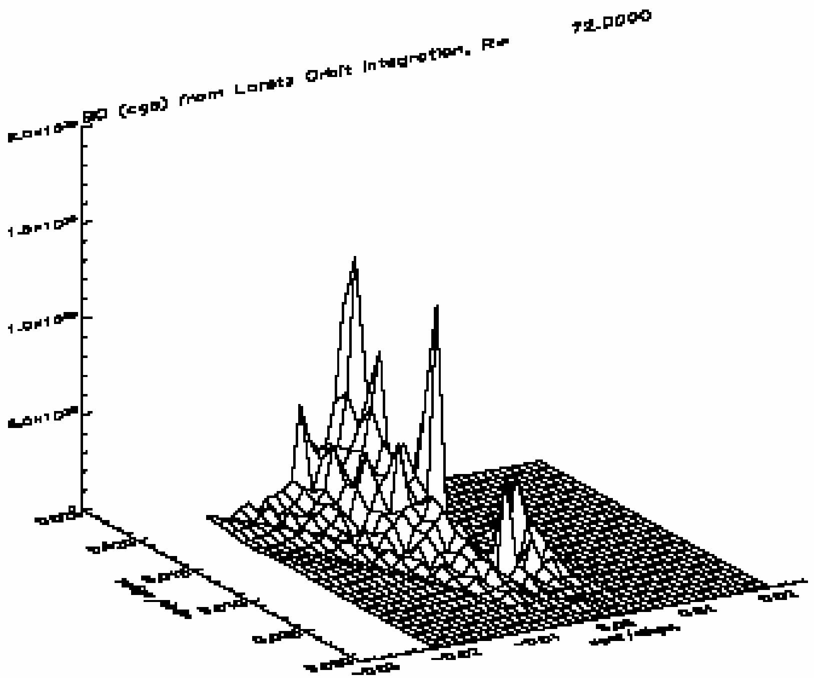
Orbit widths not negligible, even in C-Mod

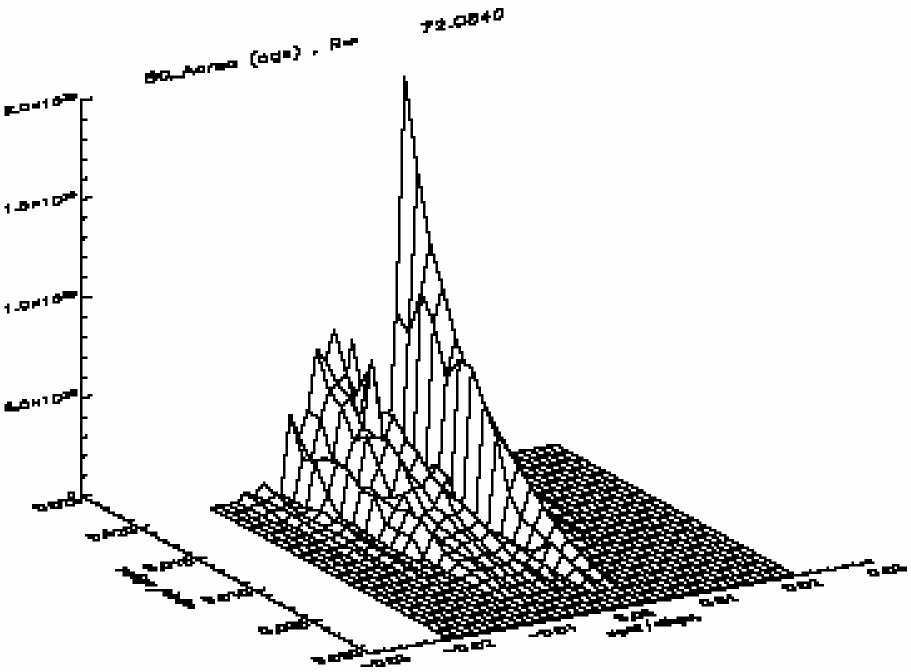
- Shown at right are trajectories for 12 particles in the C-Mod case:
  - All partciles launched from 80 cm
  - 4 equi-spaced || velocities
  - 3 equi-spaced ⊥ velocities
  - 409,600 complete poloidal orbits
- Diffusion Coefficient calculations done on CRAY XT3 (ORNL) using 256 processors @ 10 min.



Comparison of RF Diffusion Coefficients from AORSA/CQL3D and Lorentz Force Integration at **R= 72 cm**

(C-Mod minority ICRH case)

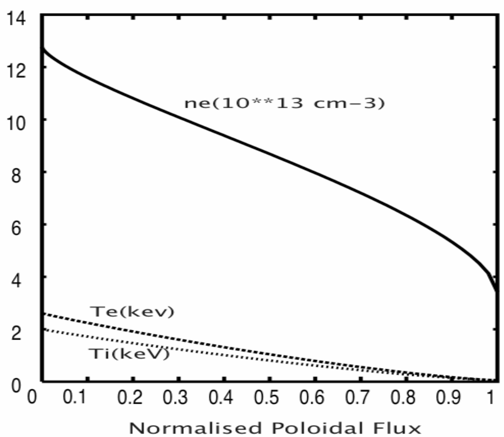


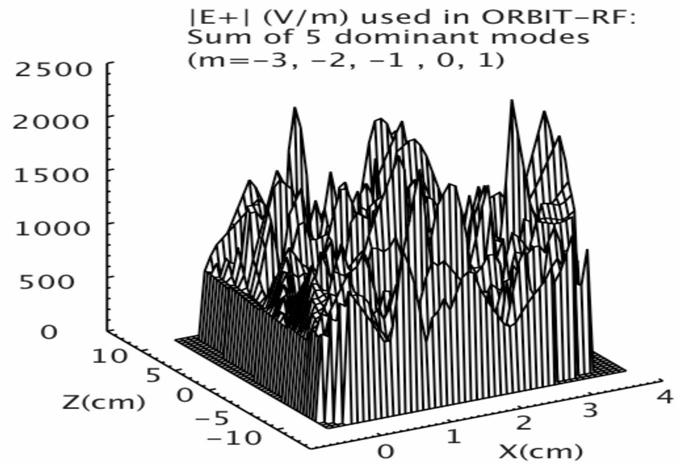


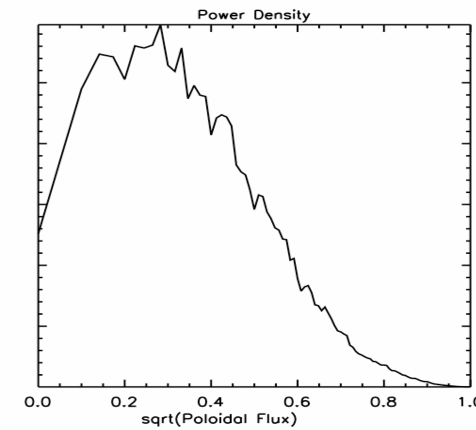
- Lorentz Orbit Code -DC
- AORSA/CQL3D

Preliminary ORBIT-RF / TORIC results indicate small orbit loss (~10%) at ICRF power level in C-Mod (0.6 MW)

10000 particles used. Simulations done for 140msec (~ 2 slowing down times)







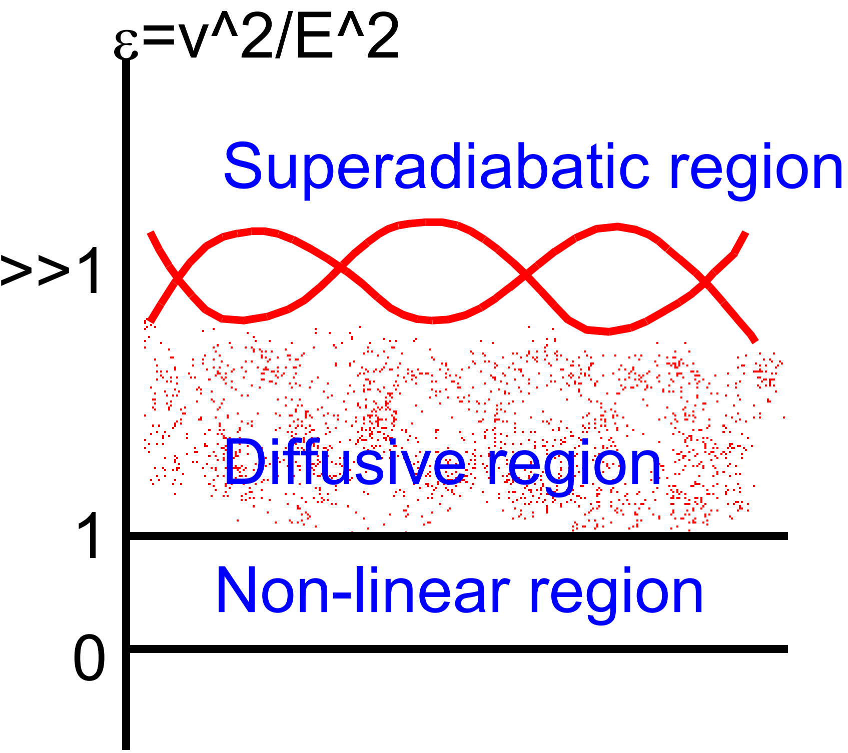
Approach used was to scale E+ field from TORIC, (keeping same spatial profile) and compute ORBIT losses:

Case1) E+(TORIC)× 50 : P(H) ~ 0.16 MW (no loss)

Case2) E+(TORIC)× 100 : P(H) ~ 0.38 MW (0.4% loss) : Results shown in Figs. above

Case3) E+(TORIC)× 200 : P(H) ~ 0.8 MW (9% loss)

Assessing the validity of QL Theory to describe ICRH in a tokamak



1. **Superadiabatic** – wave kick is too small to avoid phase locking with particle.
2. **Diffusive** – kicks are random and small- this is what is typically assumed.
3. **Non-linear** – orbits are strongly affected by waves. May or may not be still diffusive.

Simulations show that large electric field can destroy superadiabaticity via phase stochasticity

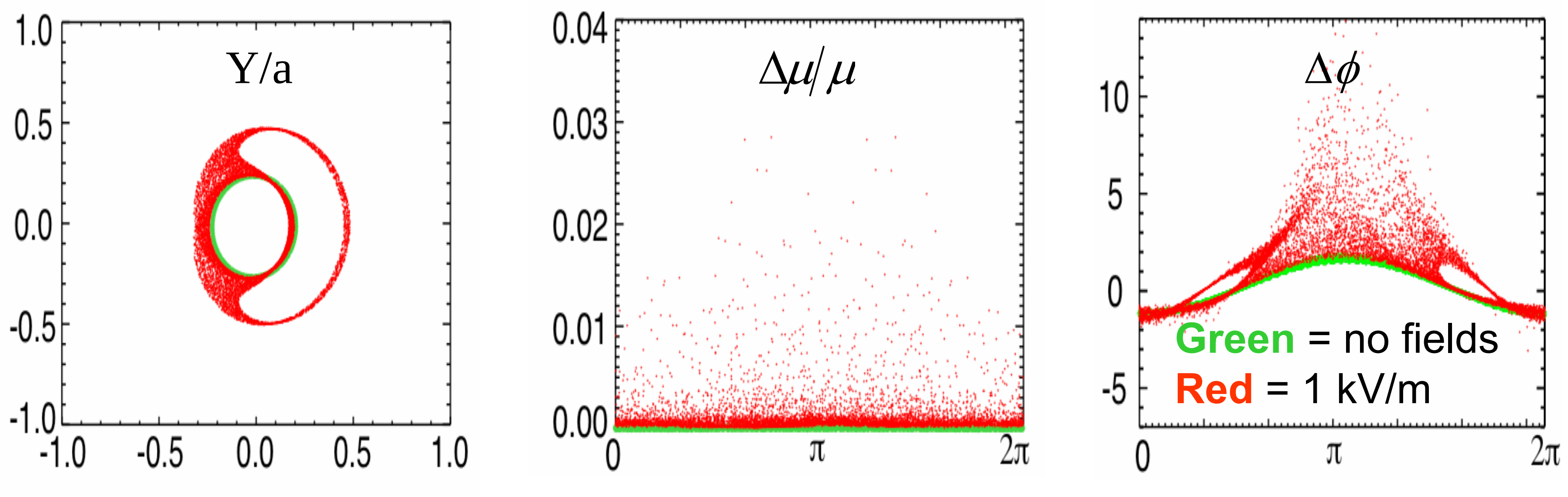
- From Stix, Chapter 17:

$$\varepsilon^4 = \frac{q^3}{64\pi} \frac{\Omega^2 v_\perp^4 r^4}{v_{//}^7 R \tau_s} \quad \text{where} \quad \frac{1}{\tau_s} = \frac{\partial W / \partial t}{n_s m_s v^2 / 2}$$

$E_{RF} \approx 1$ kV/m -> ε=0.428

Orbit-RF demonstration of phase decorrelation:

$$\Delta\phi = \frac{1}{2\pi} \int (\omega - \Omega_{ci}) \frac{ds}{v_{//}}$$

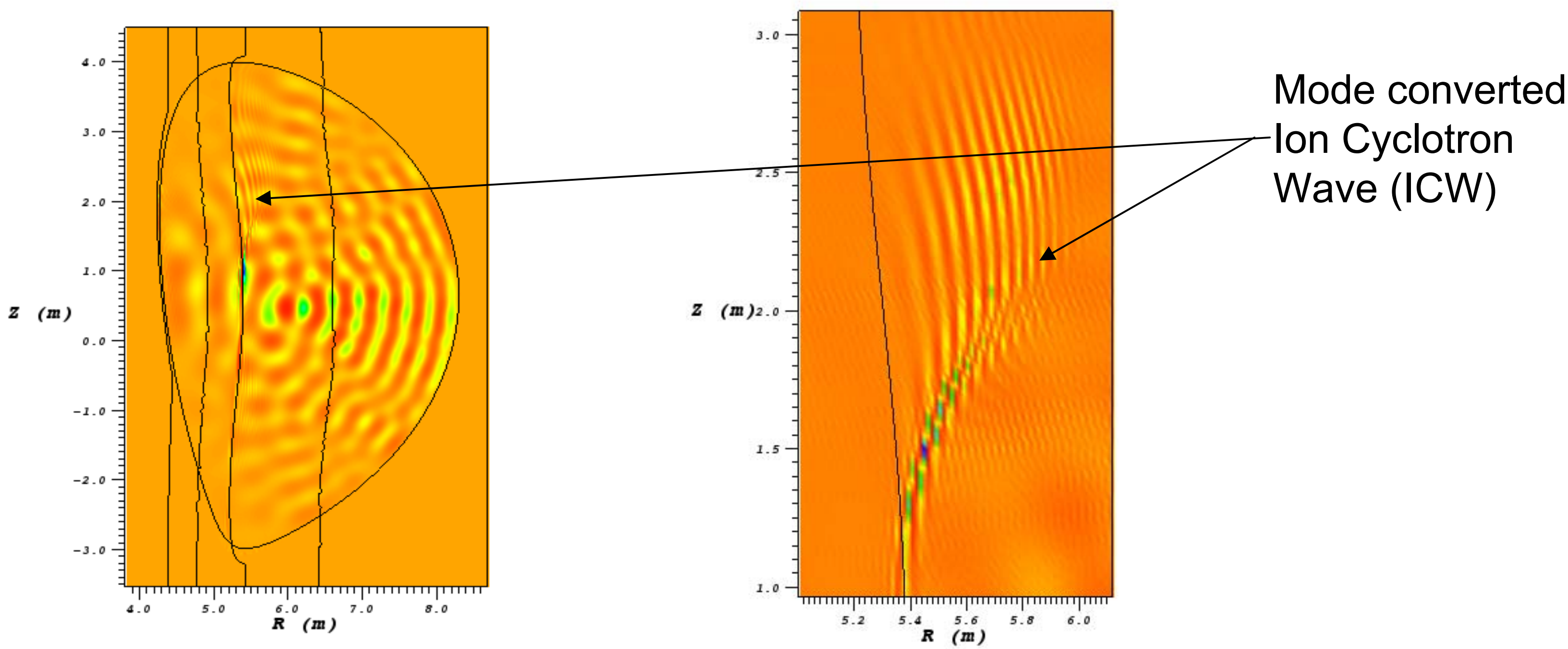


Calculations on the Cray XT-3 have allowed the first simulations of mode conversion in ITER

ITER with D:T:HE3 = 20:20:30 with $N_R = N_Z = 350$, f = 53 MHz, $n = 2.5 \times 10^{19}$ m^{-3}

(4096 processors for 1.5 hours on the Cray XT-3)

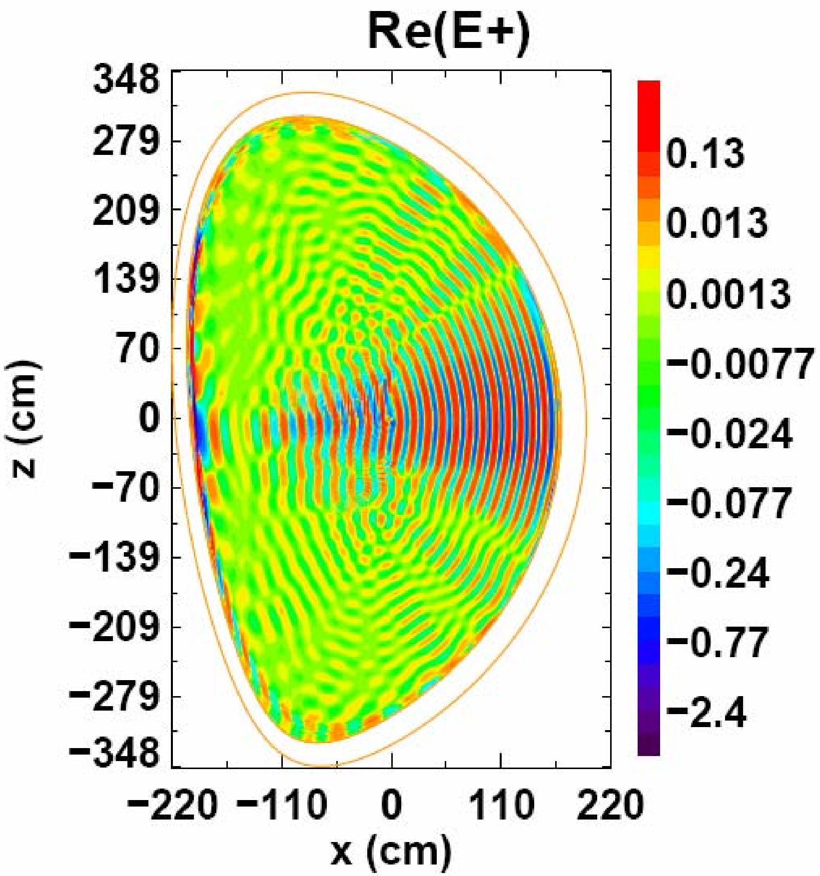
E_perp Blowup (E_parallel)

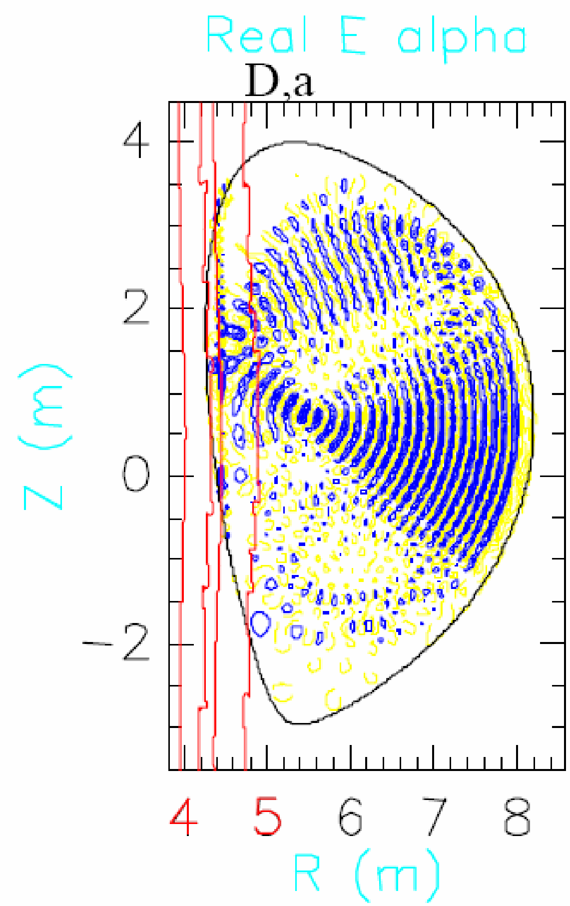


Future Work – Will extend this MC scenario to more ITER relevant densities ($\approx 7 \times 10^{19}$m^{-3})

TORIC and AORSA have been benchmarked on a $2\Omega_T$ Heating Case in ITER

Predicted electric field contours are similar





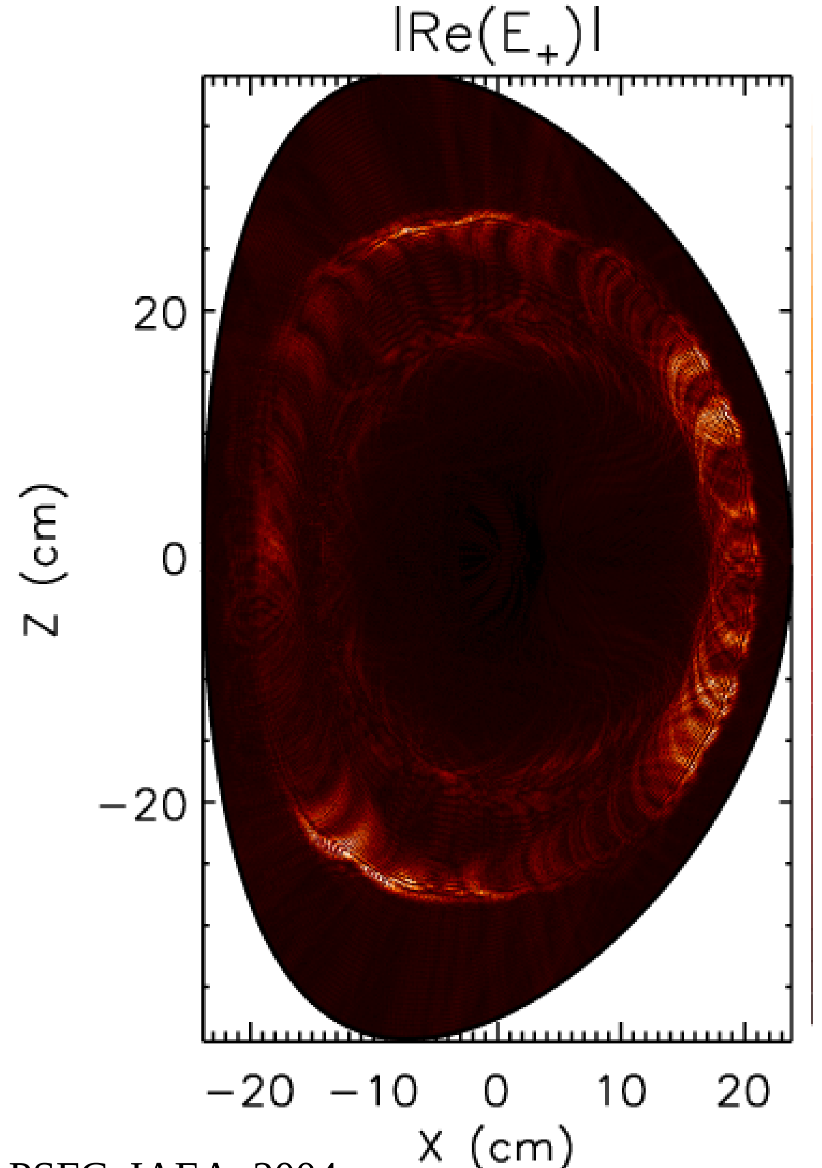
Integrated Absorption Totals for $2\Omega_T$ Heating Case in ITER

Absorption Mechanism	TORIC (Maxwellian α's)	AORSA (Maxwellian α's)	AORSA (Slowing down α's)
P(2Ω_T)	43.1 %	38.4 %	39.1 %
P(ELD)	50.4 %	45.6 %	47.0 %
P(D)	4.2 %	4.3 %	4.5 %
P(Be)	0.6 %	3.7 %	4.05 %
P(He-4)	0.41 %	2.8 %	3.0 %
P(fast-α)	0.90 %	5.1 %	2.3 %

Future Work – Need to understand reasons for differences between codes in Be, He^4, and fast-α absorption

Parallel Computing Has Made it Possible to do Full-Wave Simulations of Lower Hybrid Waves ($\lambda_\perp$ < 1 mm)

- Full-wave solver TORICLH is now being coupled to electron Fokker Planck solver (CQL3D):
  - Electron plasma response will be re-evaluated using nonthermal f_e
  - This will be the first ever combined full-wave – Fokker Planck calculation of LHCD.



J. Wright, PSFC, IAEA, 2004

For typical C-Mod parameters, the electron distribution function will have a modest plateau region

C-Mod parameters:

$T_e \sim 2$ keV

$n_e \sim 10^{14}$ cm^{-3}

$f_{LH} = 4.6$ GHz

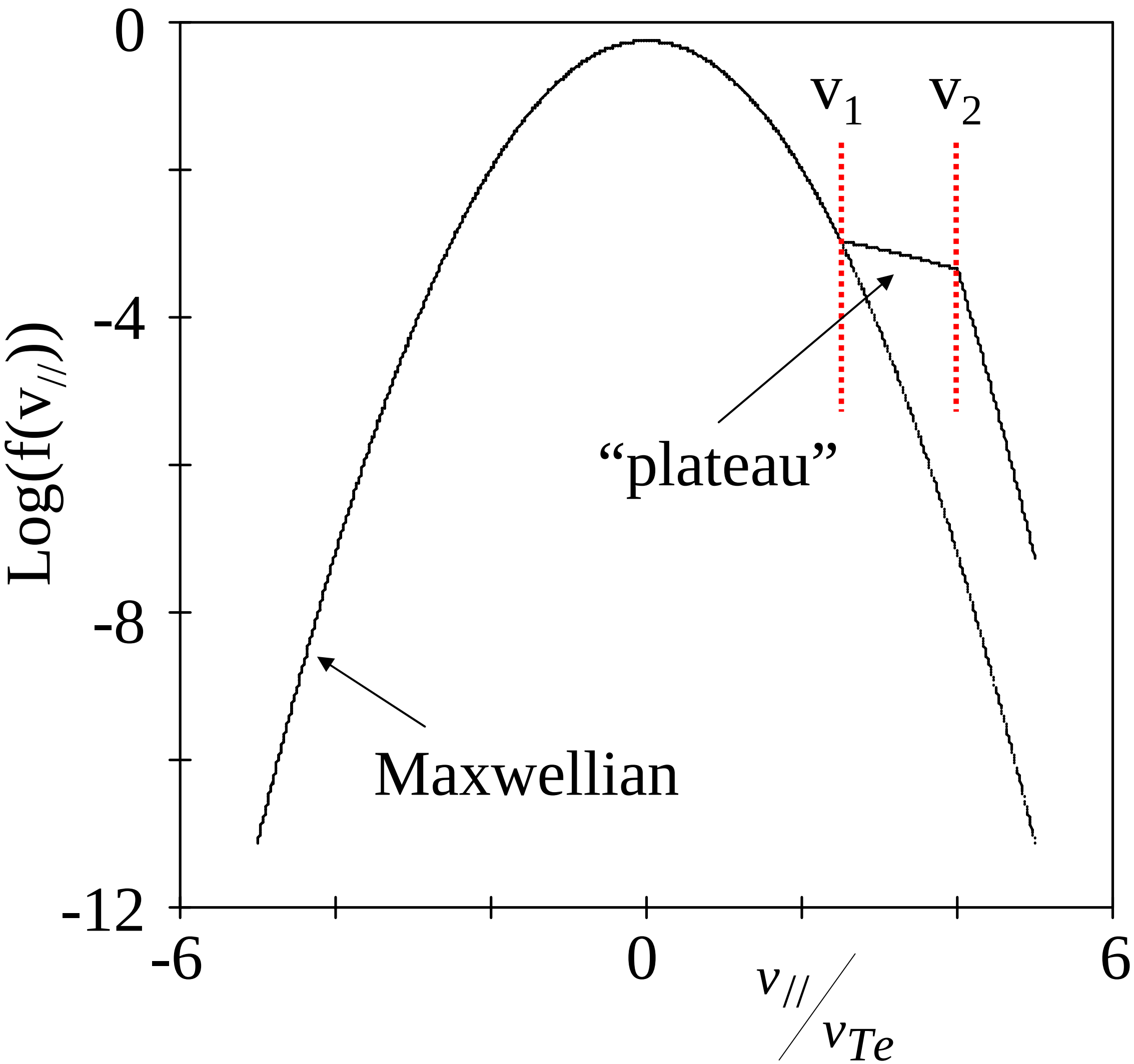
B = 5 T

$n_{//} = 2$ (launch)

"plateau":

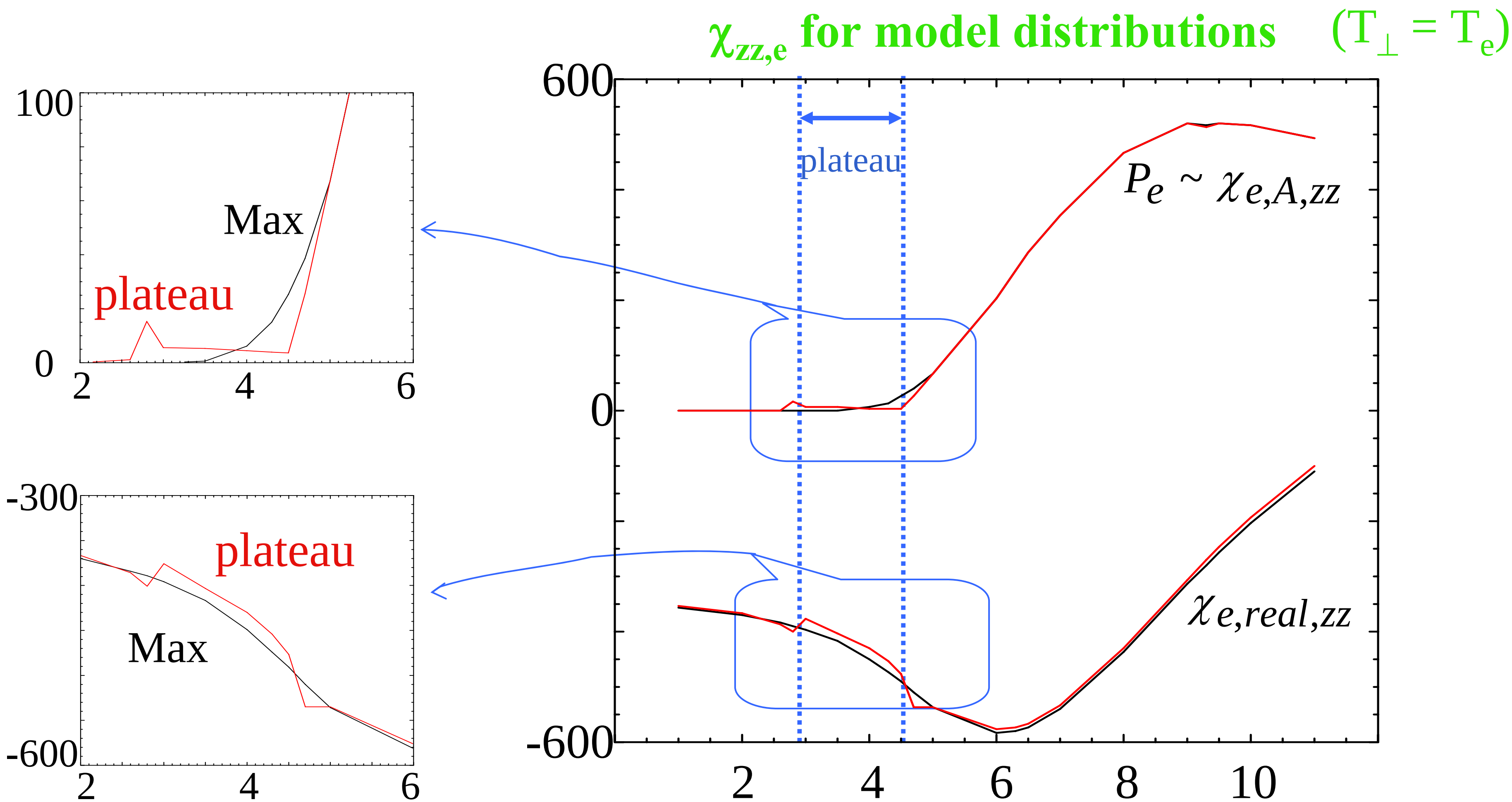
$v_1 \sim 2.5\ v_{Te}$

$v_2 \sim 4\ v_{Te}$



C.K. Phillips, APS, 2005

Modifications to the wave damping and absorption are seen in the "plateau" region of phase space



$$n_{//} = \frac{ck_{//}}{\omega} = \frac{1}{\zeta}\frac{c}{v_{Te}}$$

C.K. Phillips, APS, 2005

TORIC and AORSA can address physics effects that are missing in other fast particle mode simulation tools

Most existing simulation tools for fast particle modes are based on linear or nonlinear MHD / hybrid models that neglect or treat approximately:

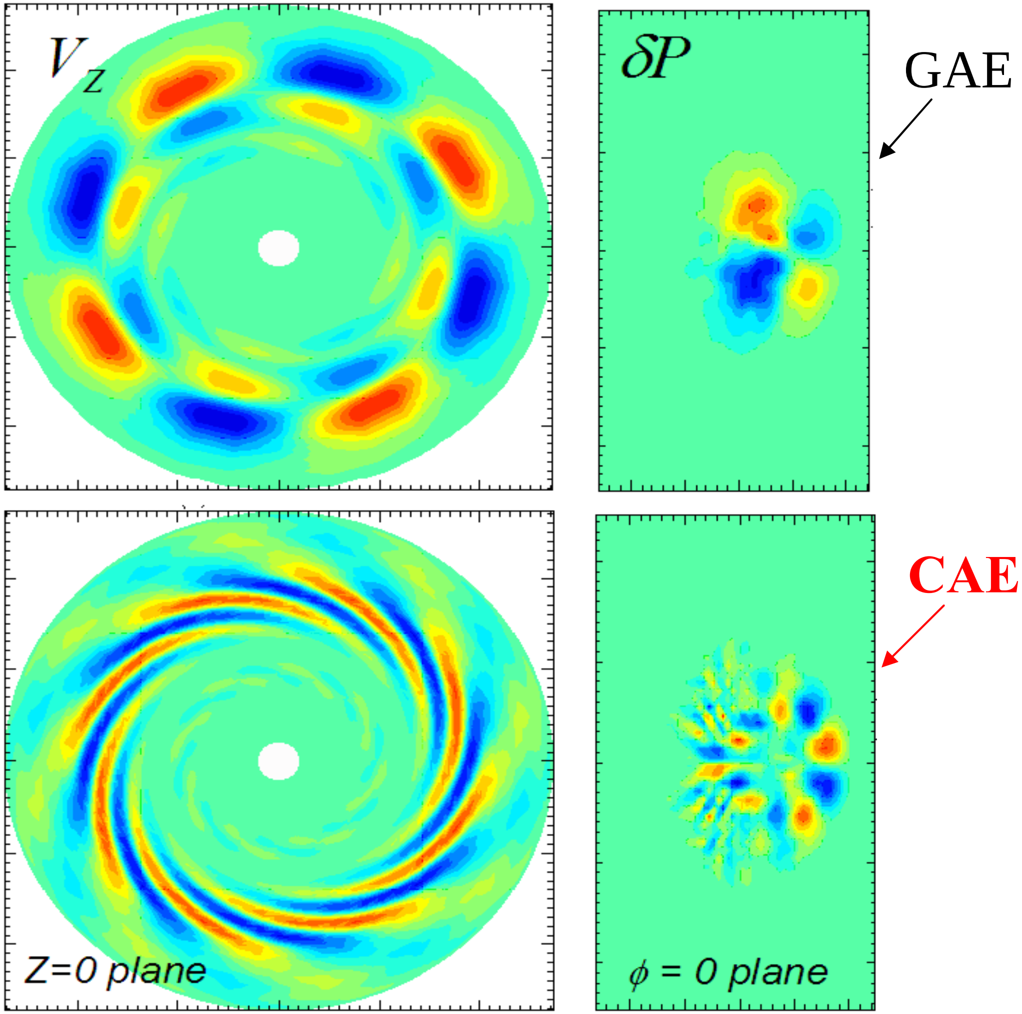
- **FLR effects, finite ω/ω_c effects, cyclotron resonances**
- **Full toroidal geometry, fast ion distributions**

⇒TORIC and AORSA retain these effects and, in addition, include much higher spatial resolution of modes, but in a linear or quasilinear treatment

⇒Approach >>> *Utilize TORIC to study dynamics of driven modes in the linear regime*

- **begin in the $\omega \sim \omega_c$ regime**
- **modify code as needed for $\omega \ll \omega_c$ regime**
- **validate code with results from driven mode experiments**

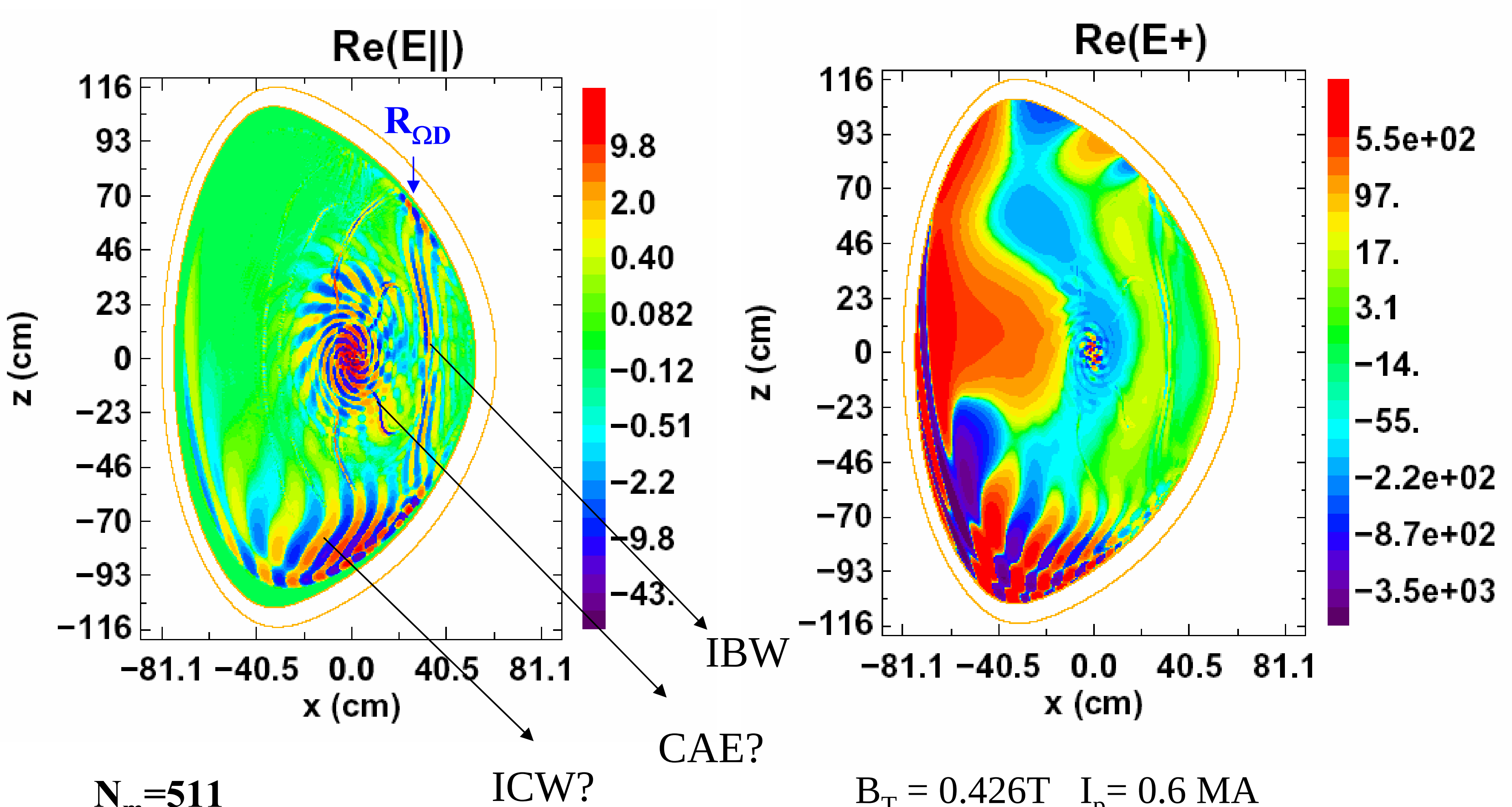
Predicted structure of fast particle modes is commensurate with TORIC resolution capabilities



HYM code simulations of GAE and CAE in NSTX (Belova)

CAE's were first predicted by the HYM code and then observed in NSTX

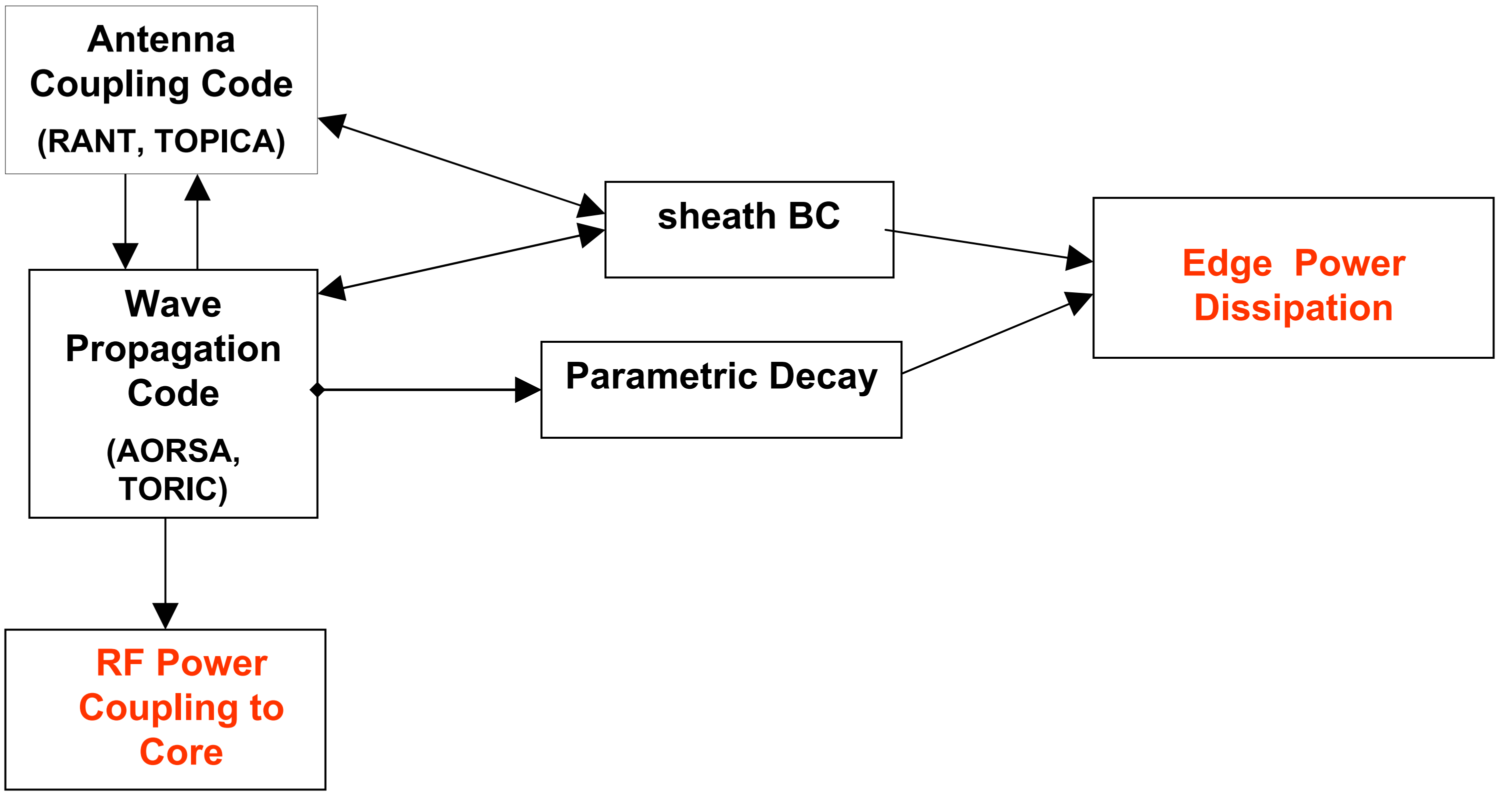
Three modes in addition to the fast wave are found in NSTX simulations with $f_0 \sim f_{\Omega D}$



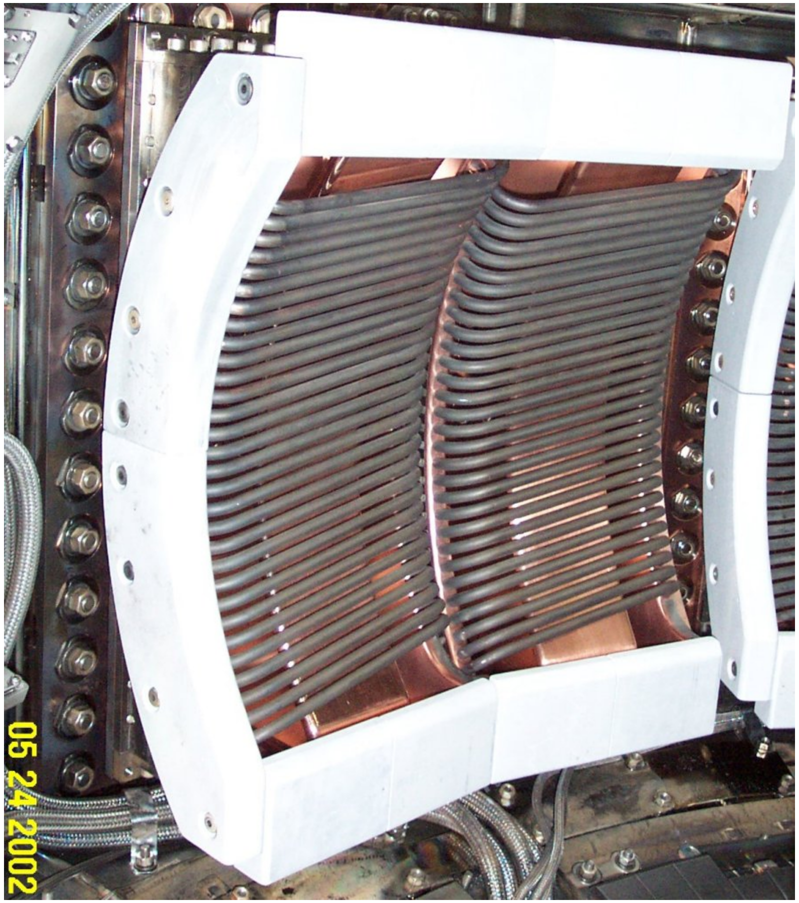
N_m=511
N_r=483

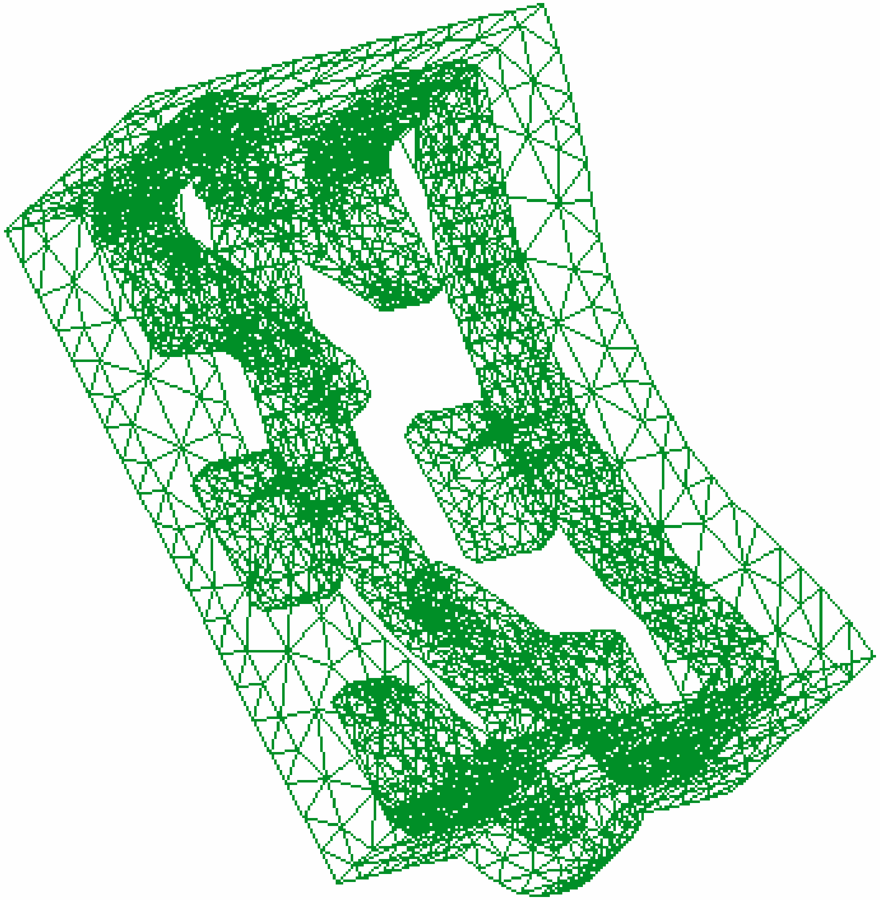
B_T = 0.426T I_p= 0.6 MA
q_a=12   f = 2.5 MHz
D-only in simulations

Long Range Goal: Integration of linear and nonlinear rf physics



Meshing for E-Port Antenna on Alcator C-Mod Using TOPICA





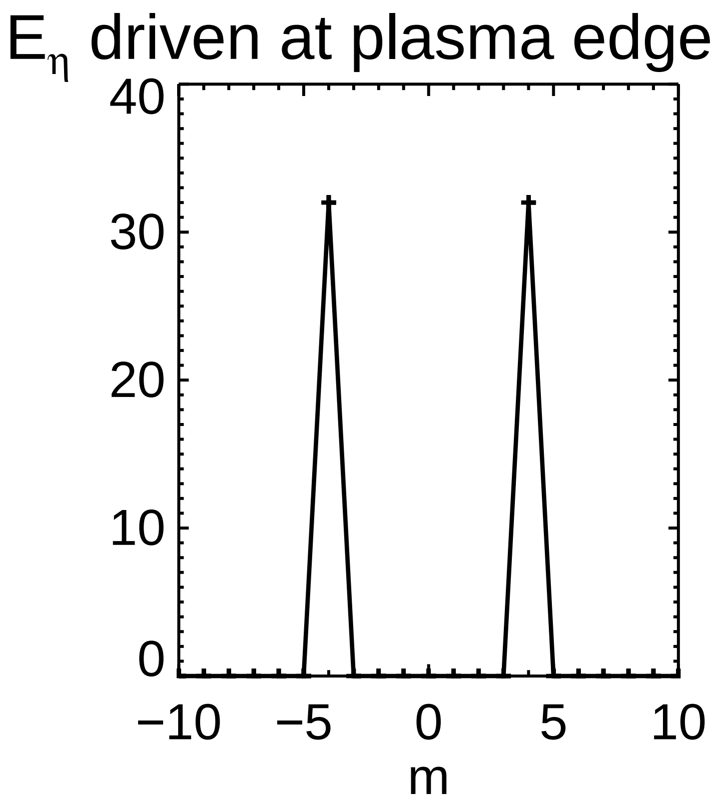
Faraday shield and backplane removed from mesh figure

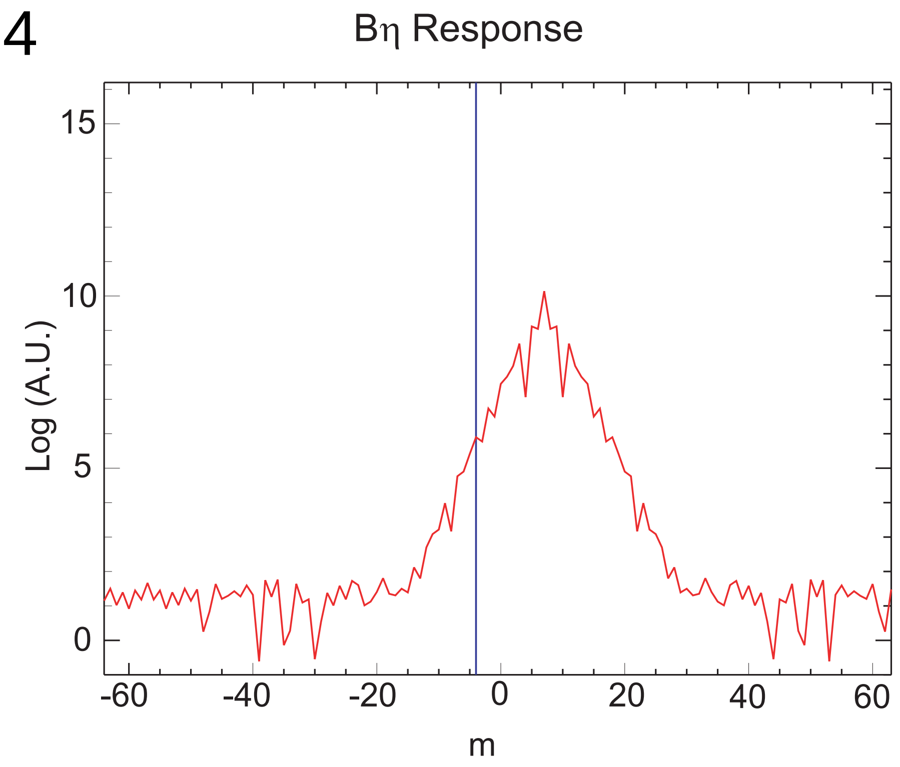
Impedance calculation is now completed

- Coupling TORIC and TOPICA codes [TOPICA (TOrino Polytechnic Ion Cyclotron Antenna):
  - Find the impedance weighted wave solution as well as the surface fields on the antenna.
- TORIC has been modified to simulate a single (m, n) excitation of a component of (E_η,E_ζ)at the plasma surface and the reactive magnetic field components are measured.
- The admittance, Y, is defined as **B** = Y**E** for the surface components of **B** and **E** where,

$$Y = \begin{pmatrix} Y_{\eta\eta} & Y_{\eta\zeta} \\ Y_{\zeta\eta} & Y_{\zeta\zeta} \end{pmatrix}$$

Modal response of TORIC system





Future Work – Next step is to pass the admittance matrix for each (m,n) excitation to TOPICA.

Nonlinear rf physics and sheath BC

- **The rf SciDAC team is presently investigating the feasibility of including a sheath BC into antenna coupling and wave propagation codes**
  - compute sheath power dissipation self-consistently
  - goal is accurate estimates of "anomalous" power dissipation, plasma heating efficiency, heating of material surfaces…

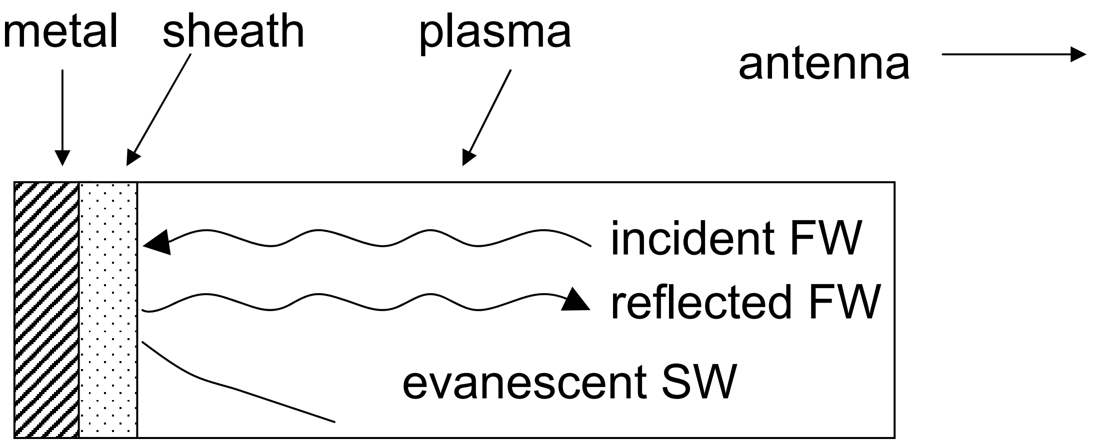
- **Derived general BC incorporating metal wall, insulating coating, and sheath (D'Ippolito and Myra, Lodestar Report LRC-06-108 (2006)**
  - incorporates rf sheath physics into the rf field solution
  - allows in principle a calculation of the spatial distribution of the rf sheath voltage and power dissipation (freq domain or time domain)

- **Sheath BC applied to a slow wave, near-field sheath problem**
  - energy conservation demonstrated by explicit analytic calculation
  - Poynting flux of propagating wave is dissipated in sheaths
  - rf E field is modified in the strong sheath limit

- **Work is underway to apply BC in a fast wave, far-field sheath problem**
  - deviation of wall from a flux surface + sheath BC $\Rightarrow$ coupling to SW
  - developing a postprocessing module for AORSA and TORIC
  - relevant to low-$k_{||}$ ICRF in tokamaks (with poor single pass absorption)

Far-field Fast Wave Sheath Solution

Wall is not a flux surface, so the FW couples to the SW to satisfy the BC at the sheath



Posed as a 3-wave coupling problem, the sheath BC gives the following solution:

$$E_1 = E_0 \frac{\mathbf{s}\cdot\mathbf{g}_2\times\mathbf{g}_0}{\mathbf{s}\cdot\mathbf{g}_1\times\mathbf{g}_2}\ , \qquad E_2 = E_0 \frac{\mathbf{s}\cdot\mathbf{g}_0\times\mathbf{g}_1}{\mathbf{s}\cdot\mathbf{g}_1\times\mathbf{g}_2}\ . \qquad \mathbf{g}_j = \hat{\mathbf{e}}_j - i\Delta\left(\mathbf{s}\cdot\boldsymbol{\varepsilon}\cdot\hat{\mathbf{e}}_j\right)\mathbf{k}_j$$

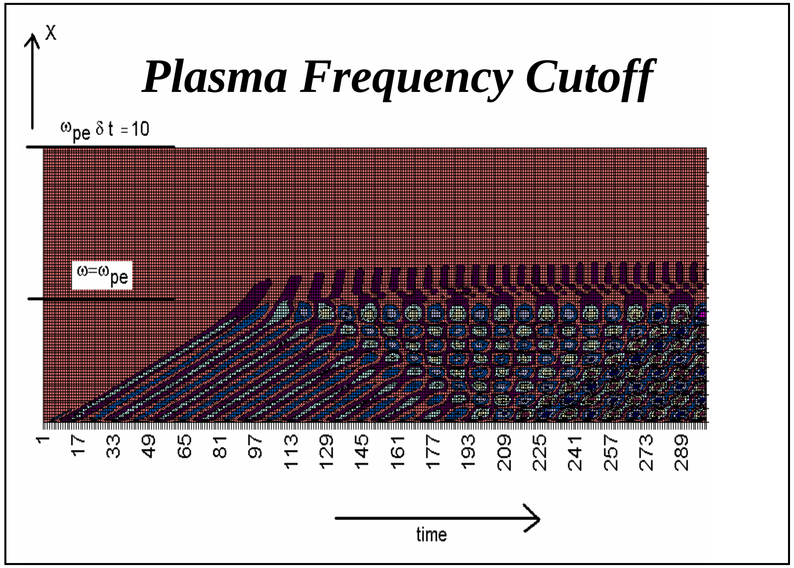
unit vector normal to sheath ($\mathbf{s}$); reflected FW (E_1); incident FW (E_0); SW (slow wave) (E_2); wavevector ($\mathbf{k}_j$); wave polarization ($\hat{\mathbf{e}}_j$); sheath width (Δ); plasma dielectric ($\boldsymbol{\varepsilon}$)

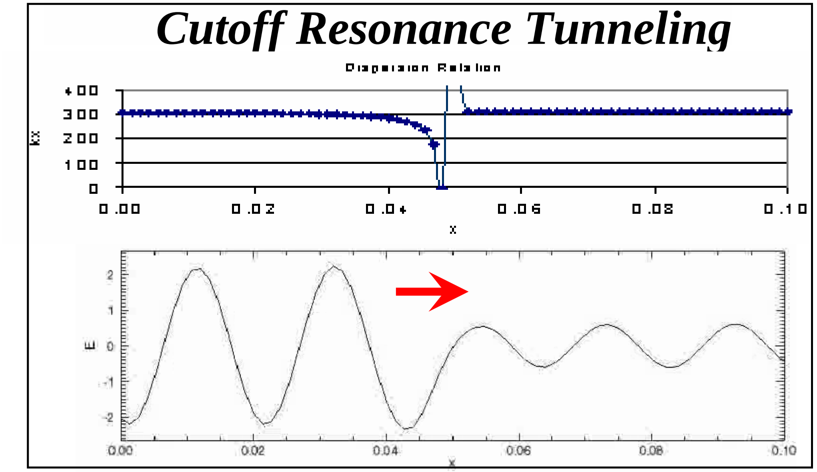
Use this solution to “post-process” the FW field solution $\Rightarrow$ sheath V and P_{sh}

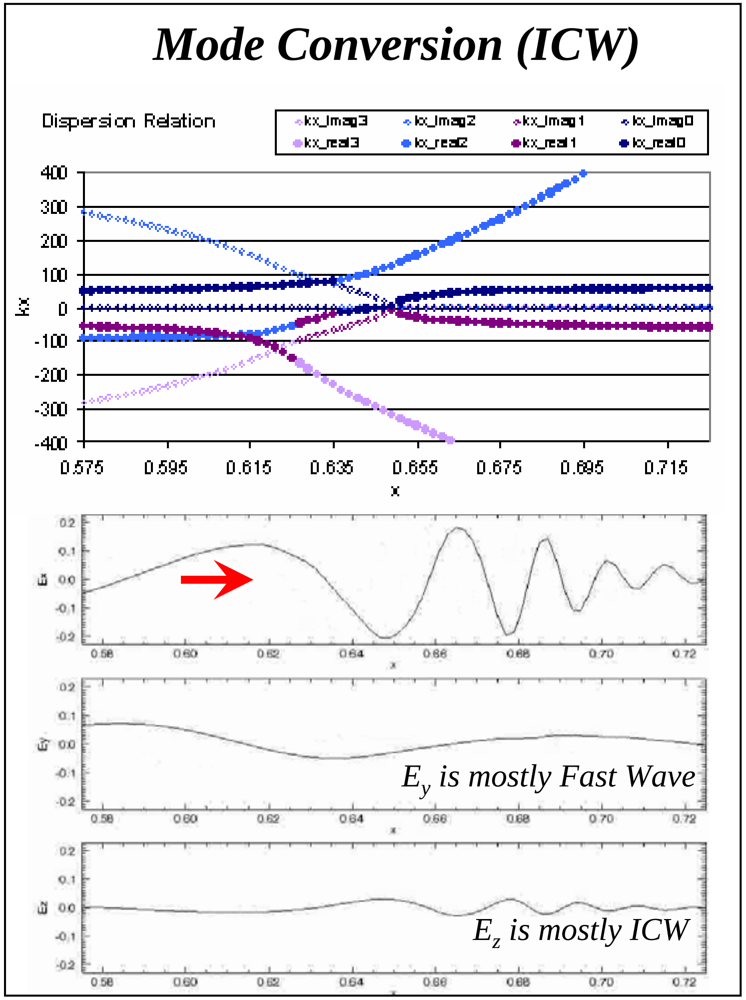
Implicit Time Domain Linear Dielectric has been Tested

- Contains all CMA diagram waves.
- Provides noise-less foundation for test-particle methods.
- Provides platform to test sheath boundary conditions.
- Is numerically stable in all pathological circumstances (cutoffs, resonances, unresolved electron plasma frequency).
- Successful demonstration (3-D, with 1-D gradients).
- Full 3-D Implementation in VORPAL software is underway.

Testing and Benchmarking of RF Time Domain

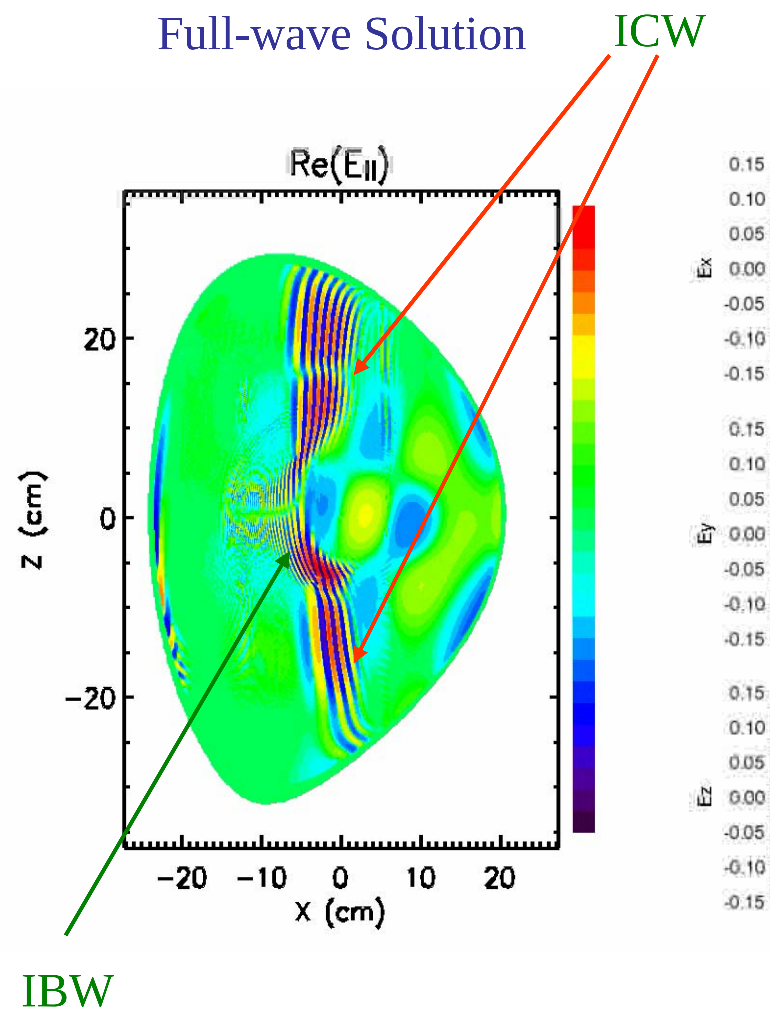




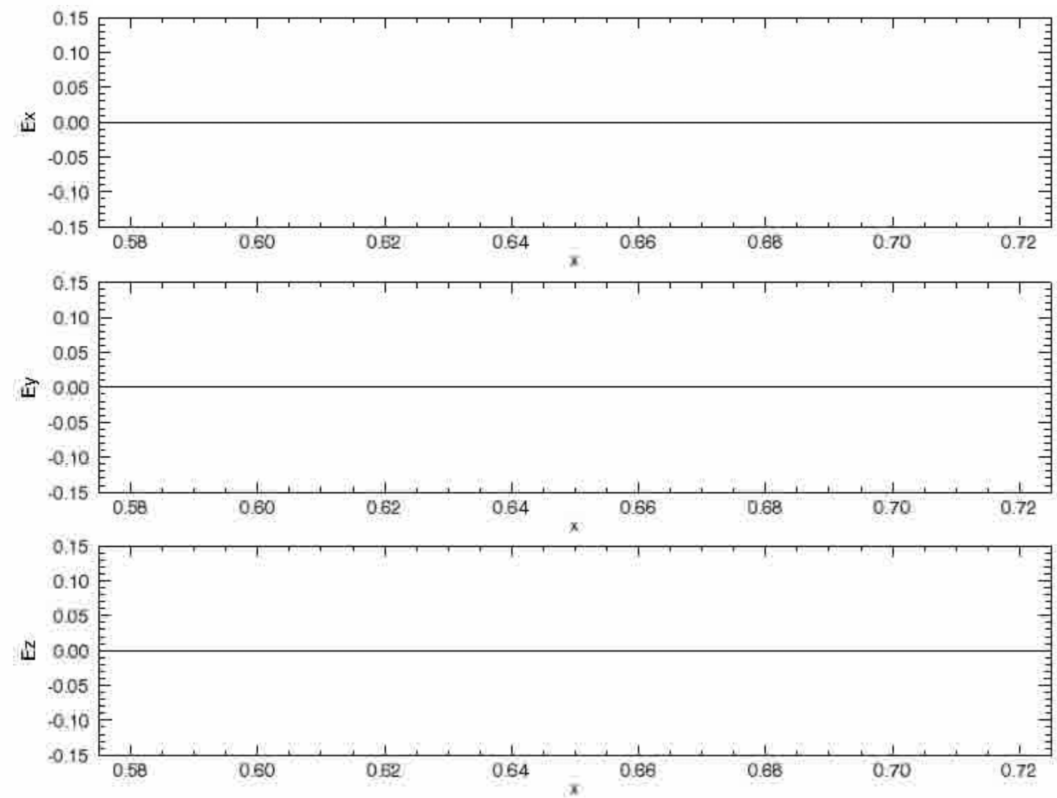


Conductivity Model has been tested on a cold plasma ICW mode conversion case -Movies

Full-wave Solution



Time Domain Solution



Summary and Future Work

- A full-wave ICRF field solver (AORSA) and bounce averaged Fokker Planck code (CQL3D)have been rigorously coupled:
  - Combined model reproduces energetic minority ion tail production in Alcator C-Mod
  - Model only partly reproduces features of HHFW – NBI interaction in DIII-D
  - Evaluation of mapping parameter for ICRH scenario indicates that conditions for stochasticity satisfied, at least up to $E_{rf} \approx 1$ kV/m.
  - Simulations of ICRF mode conversion and $2\Omega_T$ heating in ITER were performed using AORSA and TORIC.
- Finite ion orbit effects have been assessed using two methods:
  - A Monte Carlo code with an RF operator (ORBIT-RF & TORIC)
  - Via direct integration of Lorentz force equation using electric fields from AORSA (and TORIC).
  - Preliminary results indicate finite orbit width effects my be responsible for qualitative features in HHFW-NBI interaction in DIII-D.
  - Simulations for C-Mod also indicate that orbit effects could be responsible for differences between the bounce-averaged D_ql and D reconstructed from orbit integrations.

Summary and Future Work

- Future
  - Plan to re-visit DIII-D and NSTX HHFW – beam interaction experiments with careful comparison of AORSA/CQL3D and ORBIT-RF predictions.
    - Assess role of finite orbit effects and spatial diffusion.
  - Expect coupling between TORIC and CQL3D to be completed in the coming year:
    - Self-consistent simulations of minority ICRF and LHCD will then commence.
  - We will assess implementation of the “DC” code as a “call-up” module for evaluating the diffusion coefficient.
  - Simulations of driven particle modes (CAE’s) in NSTX appear promising and will continue.
  - Assessment of wavelet approach for full-wave solutions in 2D will commence shortly:
    - PPPL graduate student will work with Project during a Summer Practicum.
    - Whitepaper to be rwritten (as first proposed at summer workshop in August, 2005).