The Role of High Performance Computing in Understanding RF Wave-Particle Interactions in Fusion Plasmas

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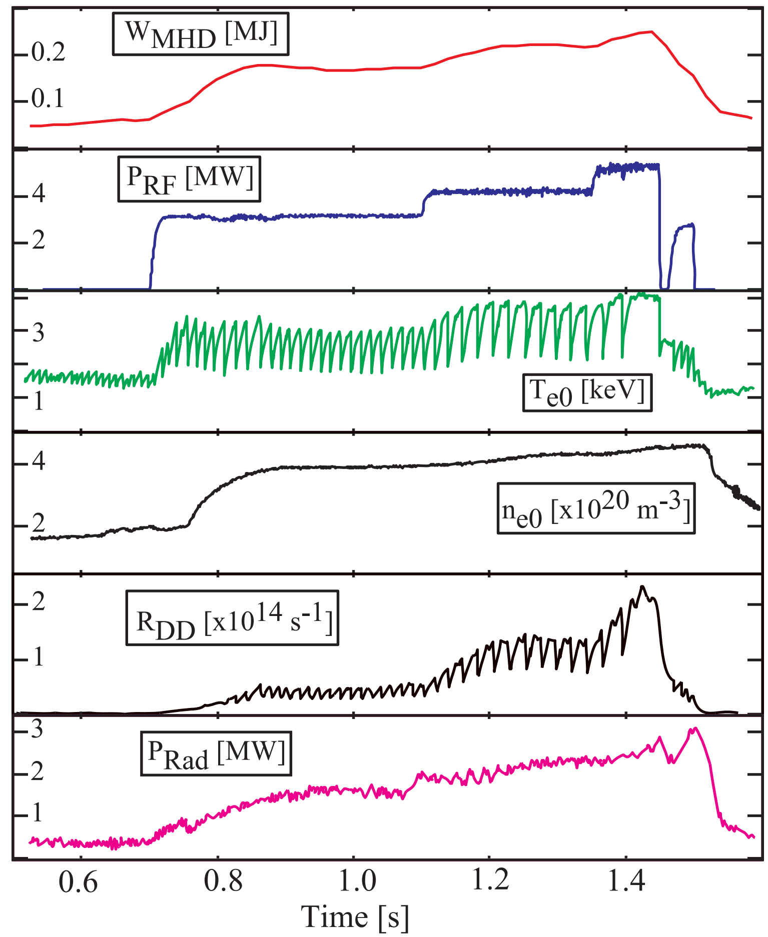
Plan for this Lecture

- Professor Saskia Mordijck just gave a general introduction to waves in plasmas
- This lecture we will concentrate only on wave-particle interactions in the ion cyclotron range of frequencies (ICRF) with a discussion of the following:
  - Advantages of ICRF power as an actuator
  - Wave dispersion characteristics
  - Equations that describe ICRF wave-particle interactions
  - Why High Performance Computers (HPC) are needed
  - Examples of how HPC has advanced our understanding [mode conversion, energetic particle effects, and interactions with the scrape off layer (SOL)]
  - Future directions - interactions with SOL and plasma-material-interactions (PMI)

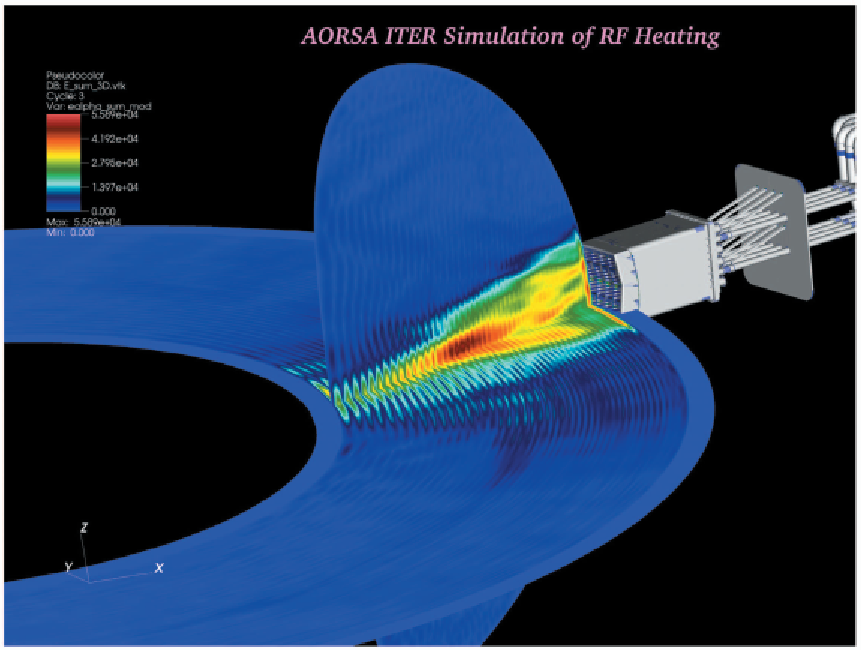
Advantages of using ICRF power as an "actuator"

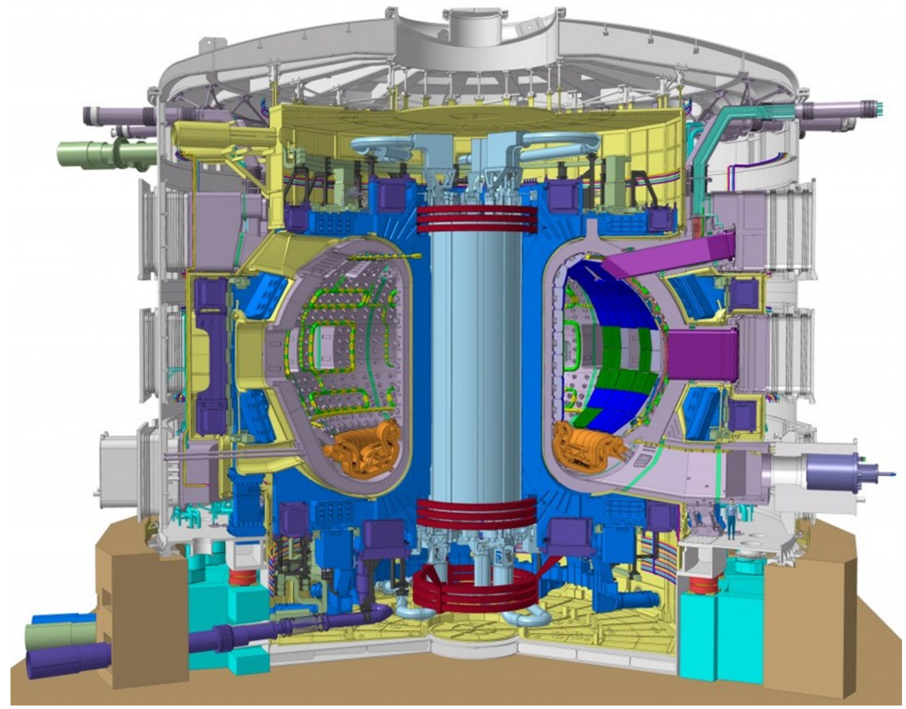
- RF source technology already exists:
  - 30-120 MHz transmitters
  - Power brought to tokamak using conventional coaxial lines
- Power is coupled to plasma using phased current straps:
  - *Antenna response in the toroidal direction can be decomposed into independent Fourier modes ~ exp(inϕ)*

- Core wave physics has been demonstrated on present day devices



ICRF power is one of the three planned auxiliary heating sources for the ITER device now under construction





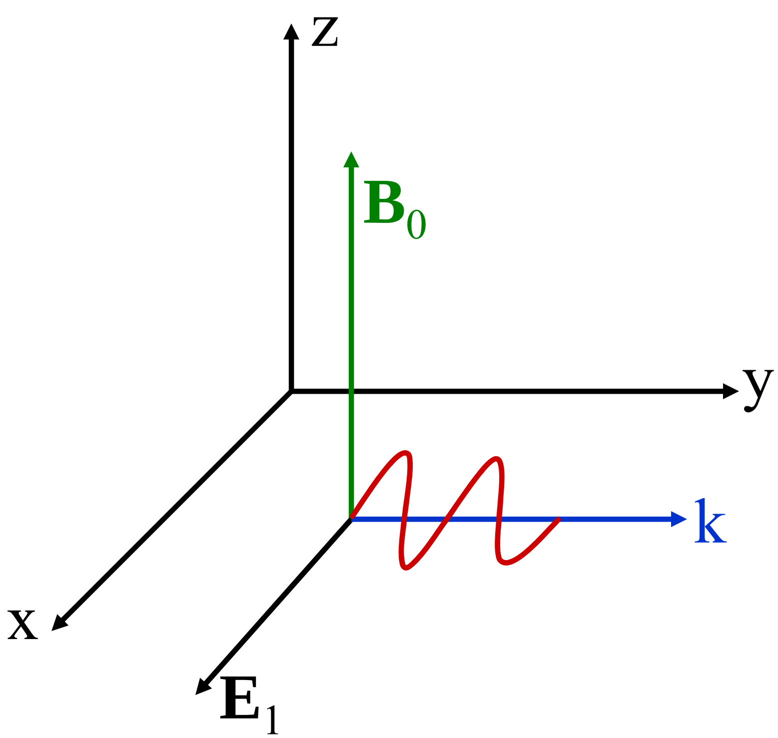
Jaeger PoP (2008)

- Limited toroidal extent of 3D electric field reconstruction clearly shows the strong absorption of ICRF waves using the second harmonic tritium ion cyclotron scheme in the ITER Scenario 2
- **ITER simulation summed over 169 toroidal modes of the antenna**
- **AORSA wave solver run on JAGUAR OLCF using 2048 processors for 8 hours of wall clock time**

Dispersion and physical characteristics of the ICRF wave

- Wave is a low frequency ($\omega \sim \Omega_{ci}$) *electromagnetic* ion mode with $\mathbf{k} \perp \mathbf{B}_0$
- $\mathbf{E}_1 \times \mathbf{B}_0$ drifts lie along k so that the plasma is compressed and released in the course of a wave oscillation →

Sometimes called a *compressional* Alfven wave



F. Chen and T. Stix - textbooks

- Dispersion relation can be derived from:
  - Two fluid momentum equations keeping pressure term
  - Continuity equation

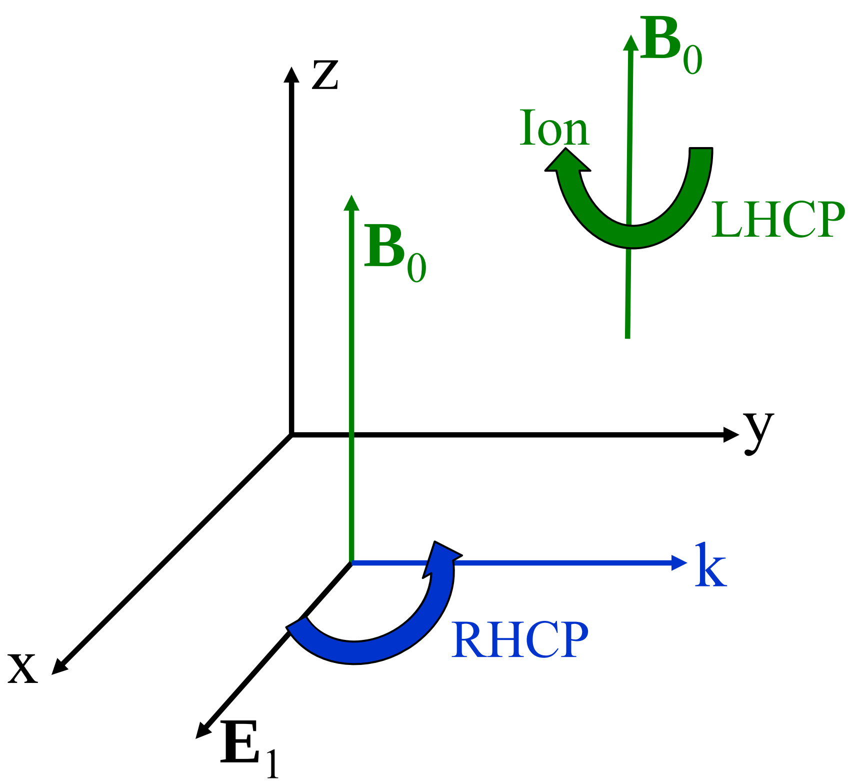
$$\omega^2 \approx k_\perp^2 \frac{v_s^2 + v_A^2}{1 + (v_A / c)^2}$$

$$v_s^2 = \gamma T_e / m_i \text{ (ion accoustic speed)}$$

$$v_A^2 = B_0^2 / (\mu_0 n_i m_i) \text{ (Alfven speed)}$$

ICRF wave polarization and impact on absorption

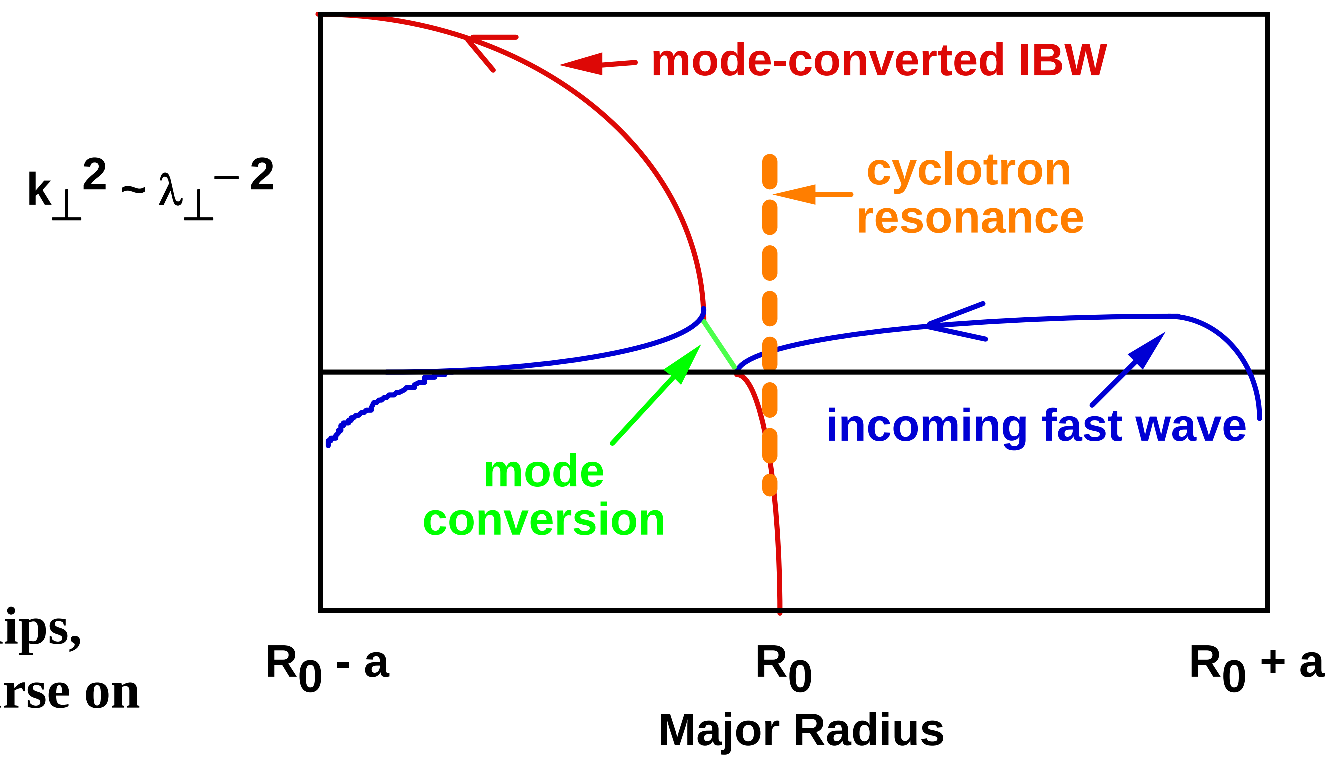
- Dispersion relation for the magnetosonic wave is not singular at $\omega = \Omega_{ci}$, and thus there is no ion cyclotron absorption at that layer
- Physically this occurs because the wave is right hand circularly polarized (RHCP) whereas the ion is left hand circularly polarized (LHCP) → thus there is no secular interaction between the ICRF wave and ion



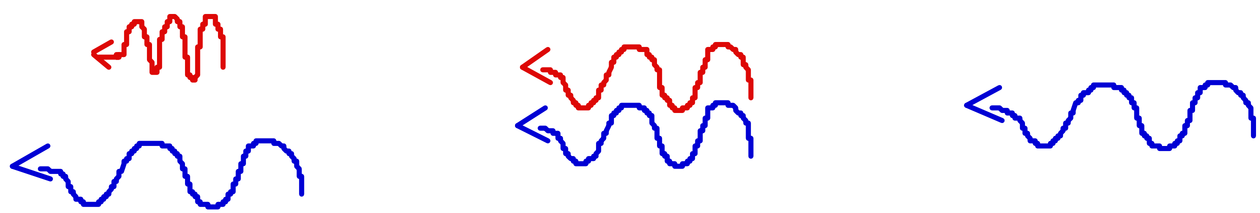
- If a dilute light "minority" ion species is added to the plasma then the wave is resonant at the minority ion resonance where $\omega = \Omega_c$(minority):
  - Wave electric field acquires a LHCP component and absorption takes place
- Two popular ICRF "minority" heating schemes:
  - Deuterium majority and hydrogen minority – D(H)
  - Deuterium majority and Helium-3 minority – D(^{3}He)

F. Perkins IEEE Trans. On Plasma Science (1984)

Introduction of minority ion species leads to the "Ion-Ion Hybrid" resonance and concomitant mode conversion to a short wavelength mode – the ion Bernstein wave (IBW)



C. K. Phillips, PPPL Course on Waves (Circa 2005)



transmitted fast wave
mode-converted slow wave

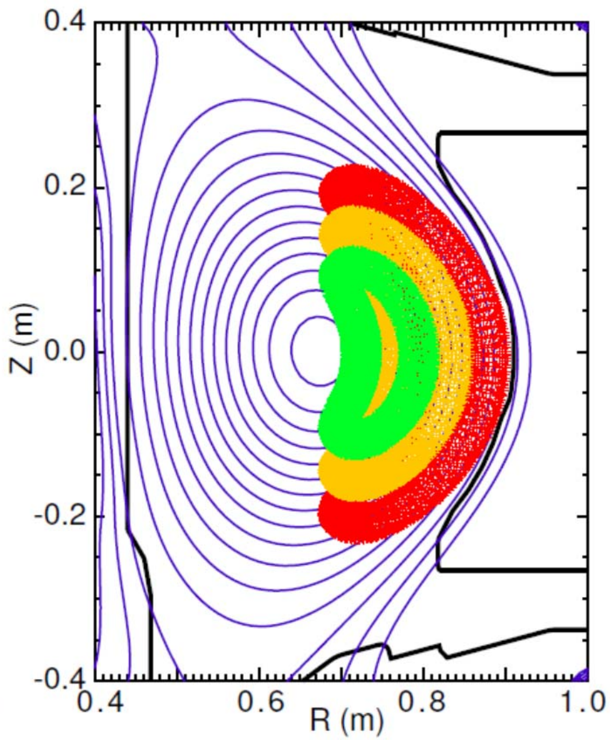
fast and slow
waves couple

incoming fast wave
slow wave cutoff

Ion cyclotron damping of the magnetosonic wave

- Ion cyclotron absorption imparts energy to minority ions in the perpendicular (to $\mathbf{B}_0$) direction → resulting in a highly anisotropic "tail" distribution:

$$\exp[-(v_{\|}^2 + v_{\perp}^2)/v_{ti}^2] \rightarrow \exp[-(v_{\|}/v_{ti})^2 - (v_{\perp}/v_{tail})^2]$$



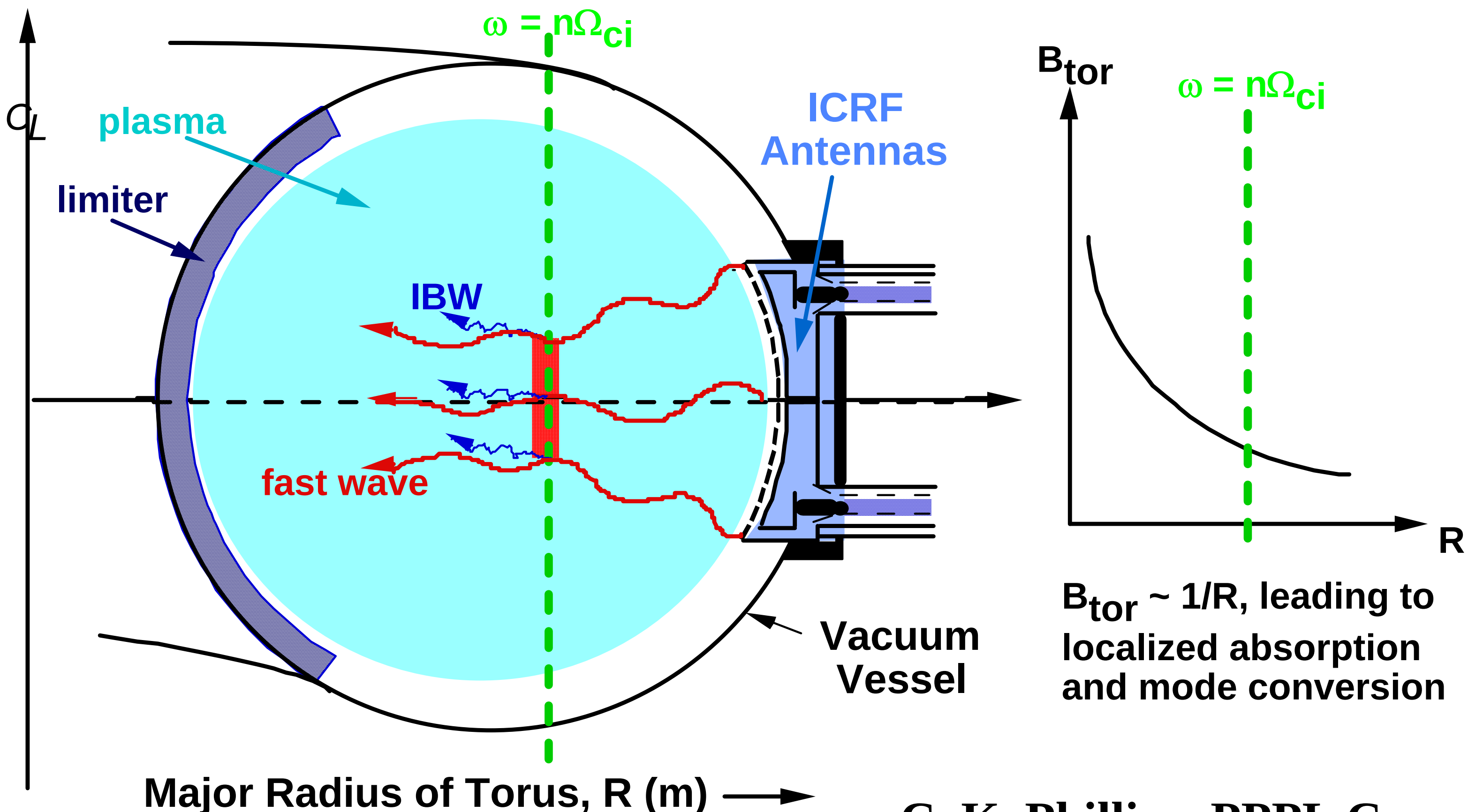
- 1 MeV ion orbits in an Alcator C-Mod plasma with 1 MA of plasma current – same R location with different Z locations. **[A. Bader, PhD Thesis, MIT (2011)**

- Characteristic bounce or "banana' motion of heated ions in the varying magnetic field of tokamak [$B_\phi \sim R^{-1}$]:
- Conservation of magnetic moment and energy during ion orbit causes $v_{//} \rightarrow 0$ at the "banana tips":

$$\mu = \frac{\frac{1}{2} m v_{\perp}^2}{B}, \qquad E = \mu B + \tfrac{1}{2} m v_{\|}^2$$

ICRF Heating Involves Three Important Processes:

- Ion cyclotron absorption with nonthermal ion tail production:
  - Consequence of FW damping on a dilute (few percent) minority ion population
- Conversion of fast wave to short wavelength ion Bernstein wave (IBW)
- ICRF antenna coupling



C. K. Phillips, PPPL Course on Waves (Circa 2005)

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 Solvers - (AORSA, TORIC)

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

$$\frac{\partial}{\partial t}(\lambda f_0) = \nabla_{\mathbf{u_0}} \cdot \Gamma_{\mathbf{u_0}} + \langle\langle S \rangle\rangle + \cancelto{0}{\langle\langle R \rangle\rangle} \text{ where } \nabla_{\mathbf{u}} \cdot \Gamma_{\mathbf{u}} = C(f_0) + Q(\mathbf{E}, f_0)$$

Plasma Response (CQL3D sMC, ORBIT RF)

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

Typical ansatz for the wave E-field yields a well-defined matrix structure

$$\underline{\underline{A}} = \begin{pmatrix} \mathbf{D} & \mathbf{U} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{L} & \mathbf{D} & \mathbf{U} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{L} & \mathbf{D} & \mathbf{U} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{L} & \mathbf{D} & \mathbf{U} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L} & \mathbf{D} \end{pmatrix}$$

$$E(x) = \sum_m E_m(r)\exp(im\theta + in\phi)$$

ϕ - symmetry assumed.

$E_m(r)$ represented by FE's

Matrix is inverted with scalable (parallel) linear algebra library that performs an LU decomposition of the matrix → ScaLapack

- **Matrix is block tridiagonal.**
- Blocks **L, D, U** are each dense matrices of size $(2 \times 3 \times N_m)^2$.
- Total of N_r block rows
- **For N_r =960, N_m = 1023, matrix size is ~ 1.1×10^{11} elements.**

What is a "High Performance Computer" ?

- A cluster of processing units (cpu's) performing arithmetic simultaneously (in parallel) at the rate of about 10^{15} (**P**eta) **f**loating **p**oint **o**perations **p**er **s**econd (flops/s).

- Maximum theoretical flop-rate (R_{flop}) is:

$$R_{flop} \approx (0.5 - 2.0)\, R_{cpu} \times N_{cpu}$$

where:

R_{cpu} is the processor clock speed (Hz)

N_{cpu} is the total number of processors

First Supercomputers were only a single or a few cores

- **Original CRAY1 "supercomputer" was capable of 133 Mflop/s !**
  - R_{cpu} = 80 MHz
  - Contained a single CPU capable of vector arithmetic (array manipulations in a single clock cycle).

- **Today, CPU's are very fast - and inexpensive !**

  $R_{cpu} \approx 2.6$ GHz

  $N_{cpu} = 1\text{-}4$ (a desktop computer)

  $R_{flop} \approx 5$ Gflop/s

Smaller computing clusters have become an important part of the HPC "ecosystem"

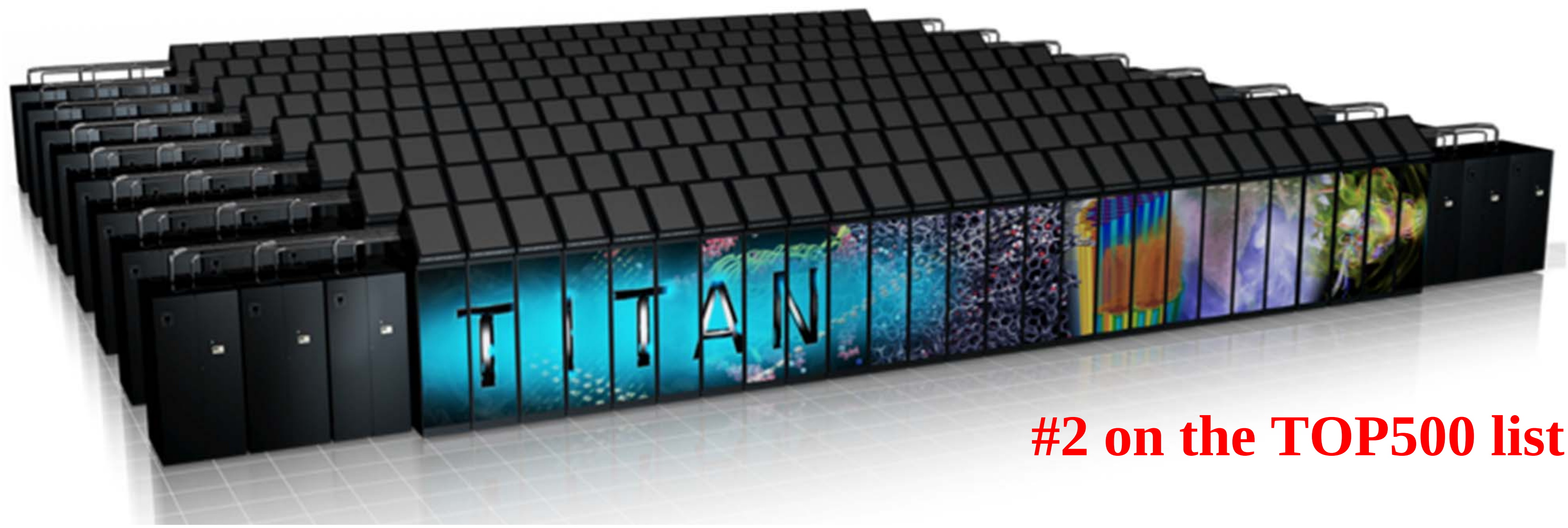
PSFC has the "Loki" Computing Cluster

- R_{cpu} = (2.1, 2.4) GHz
- 0.94 TB in-core memory
- N_{cpu} = 600
- $R_{flop} \approx$ 1-2 Tera-flop
- Configuration:
  - 75 nodes
  - 8 cores / node
- Infiniband amd Ethernet switches.

Newest Peta-scale Computer at NERSC is the CRAY XC30 named “Edison”

- R_{cpu} = 2.4 GHz
- 332 TB in-core memory
- N_{cpu} = 133,824
- $R_{flop} \approx$ 2.57 Pflop/s (peak)
- **Configuration:**
  - **5576 compute nodes**
  - **24 cores / node**

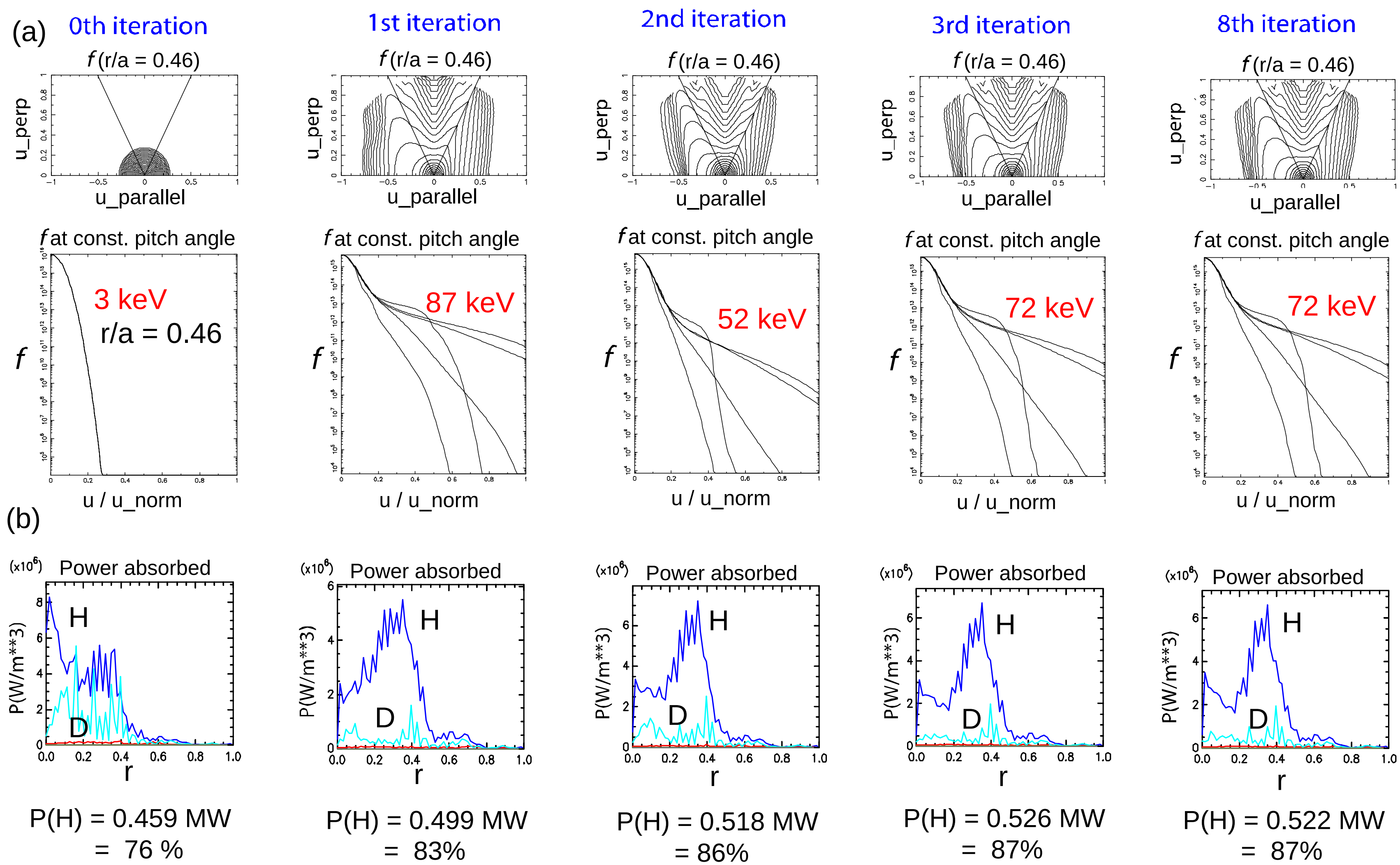
Newest Leadership Class supercomputer at ORNL ("Titan") is a CRAY XK7 which has a "heterogeneous" architecture



#2 on the TOP500 list

- 18,688 AMD Opteron 6274 16-core CPUs
- 18,688 Nvidia Tesla K20X GPUs
- **Speed: 17.59 PetaFLOPS (LINPACK benchmark)**
- **27 PetaFLOPS theoretical peak**
- **Consumes 8.2 MW of power !**

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

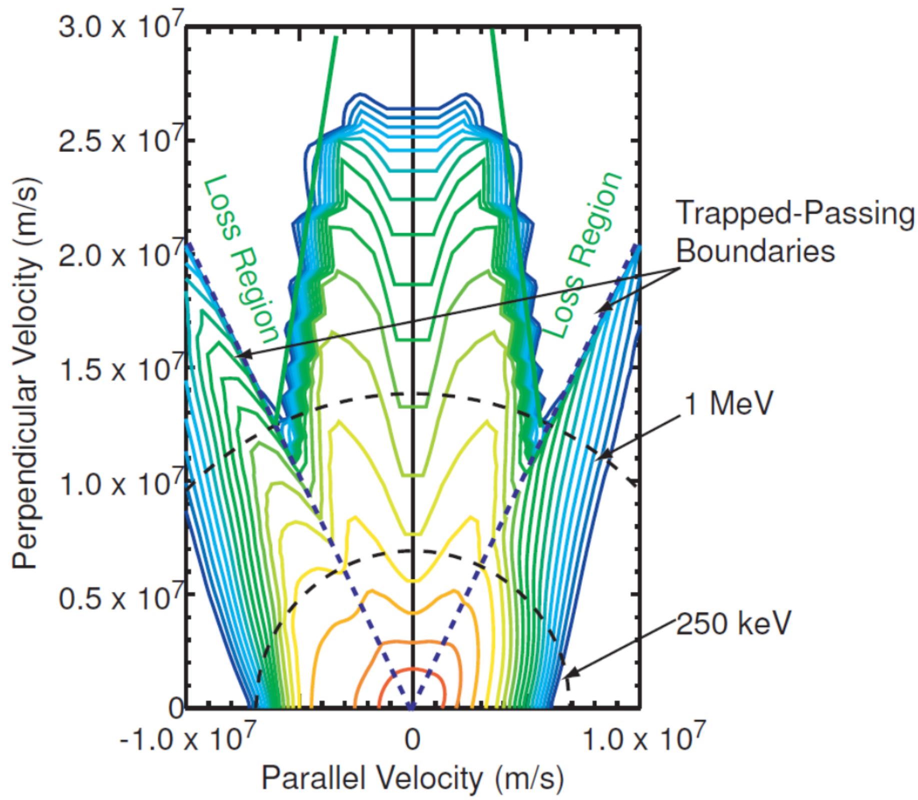


E. F. Jaeger PoP (2006)

Anatomy of an ICRF-generated fast ion tail

- Ion cyclotron absorption imparts energy to minority ions in the perpendicular (to $\mathbf{B}_0$) direction → resulting in a highly anisotropic "tail" distribution:

$$\exp[-(v_{\|}^2 + v_{\perp}^2)/v_{ti}^2] \rightarrow \exp[-(v_{\|}/v_{ti})^2 - (v_{\perp}/v_{tail})^2]$$



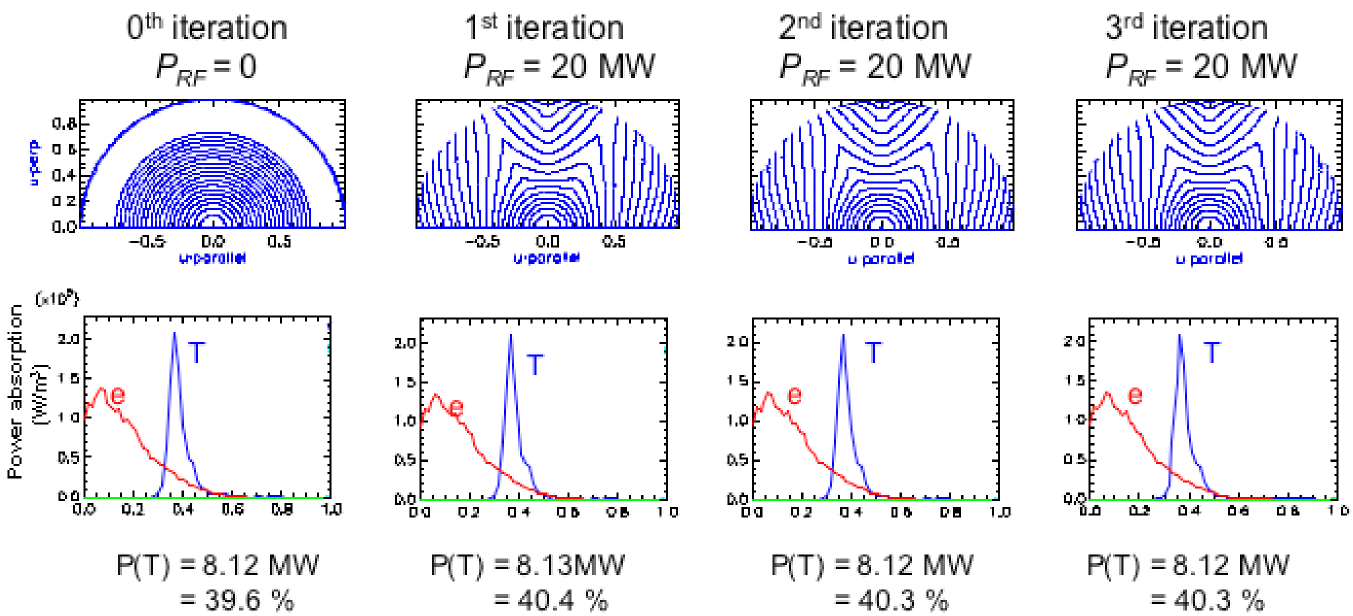
- Characteristic "rabbit ears" in distribution result from perpendicular energy gain from ICRF heating
- Energetic ions that are trapped have their banana tips (where $v_{//} \rightarrow 0$) at the resonance layer.

$$\mu = \frac{\frac{1}{2} m v_{\perp}^2}{B}, \qquad E = \mu B + \tfrac{1}{2} m v_{\|}^2$$

A. Bader PhD Thesis MIT (2011)

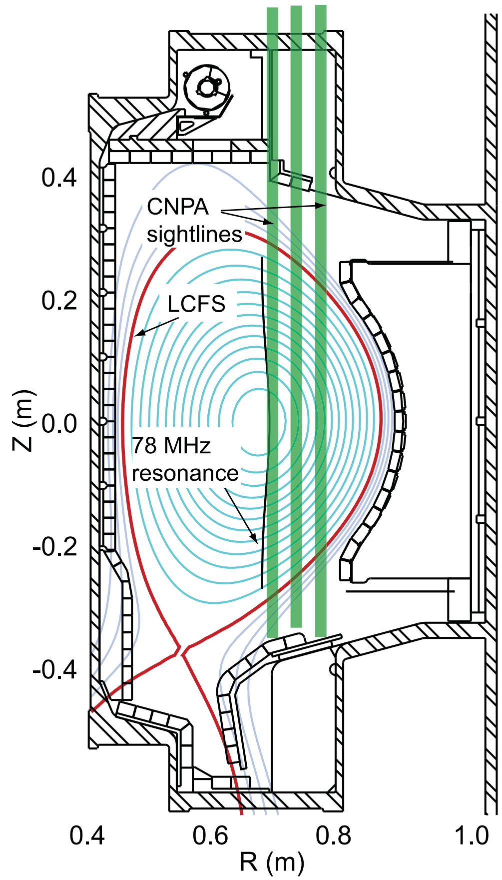
Iterated full-wave / Fokker Planck simulations have been performed for the ITER Steady State Scenario 4

ITER-AT (Snowmass) with a 50-50 DT mixture and 2nd harmonic T

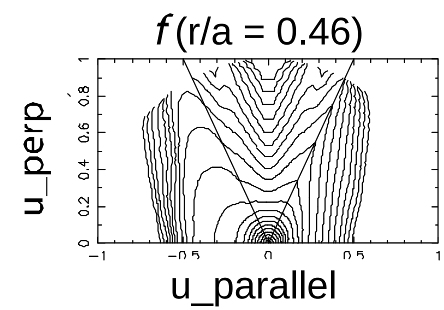


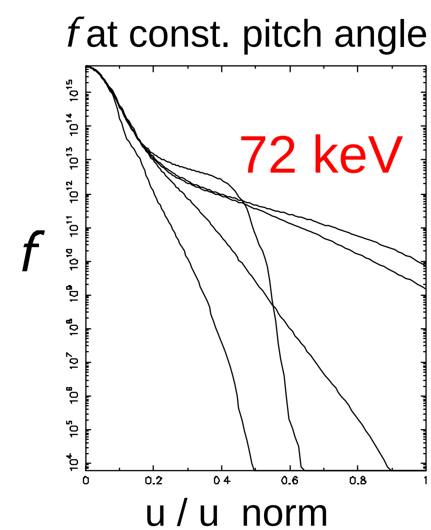
- For 50-50 DT plasma the tritium tail is weak and has little effect on the electron absorption in the ICRF heating scheme envisioned for ITER → second harmonic tritium cyclotron damping plus direct electron Landau damping
- Tritium tail formation could affect the neutron rate
- For ICRF wave absorption on fusion alphas the effect could be stronger

As an ICRF-generated minority ion tail slows down it charge exchanges with background plasma ions producing an energy dependent spectrum of photons that can be detected



- **Nonthermal minority hydrogen distribution from AORSA-CQL3D simulation are used to reconstruct a synthetic CNPA signal.**



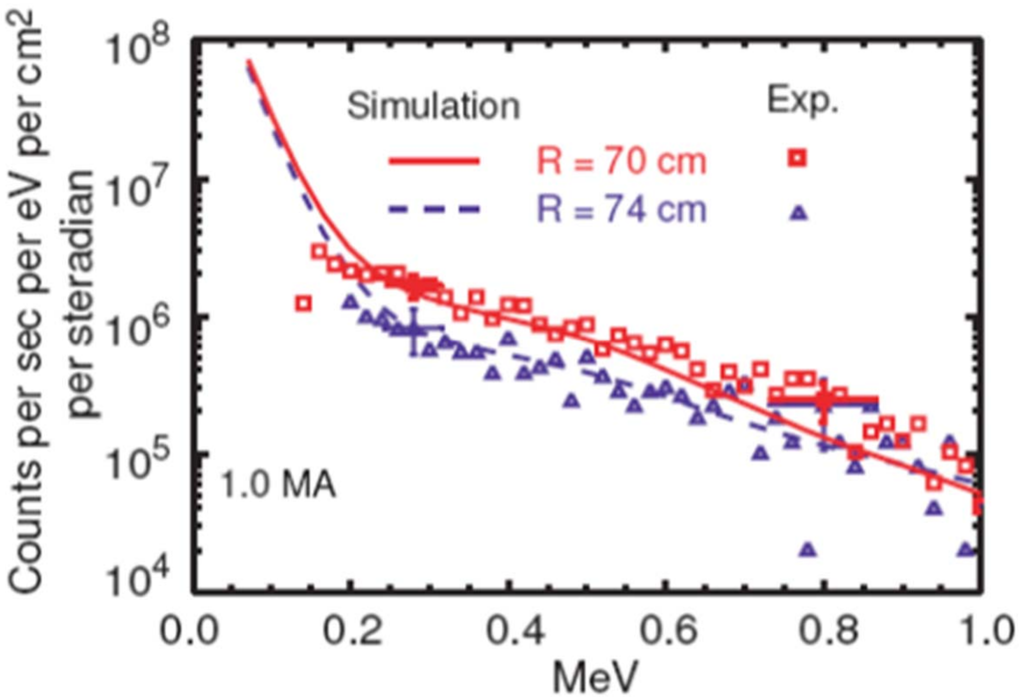


Vertically viewing chords on a compact neutral particle analyzer (CNPA) detect photon counts during ICRF minority heating.

Bader, NF (2012)

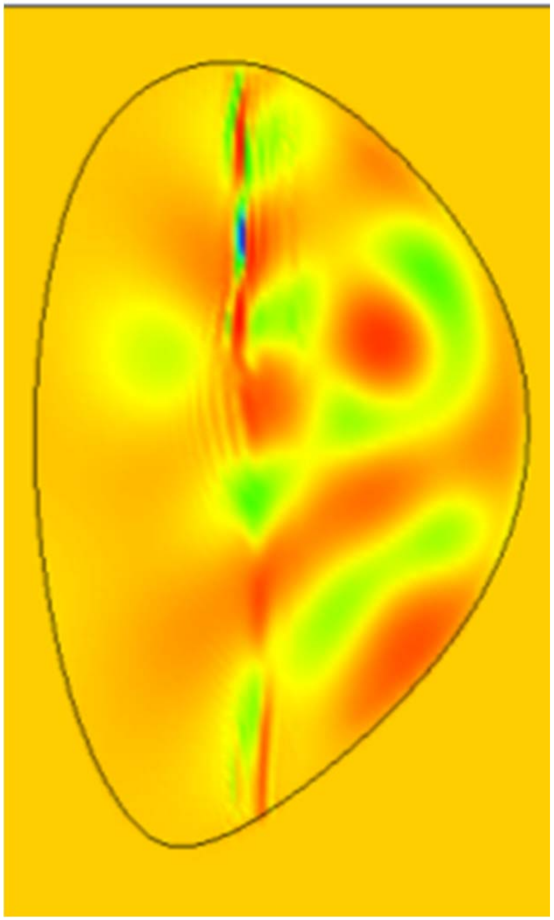
Synthetic diagnostic for CNPA has been used to validate the non-thermal ion distributions simulated by an iterated full-wave / Fokker Planck solver (AORSA/CQL3D)

- **ICRF minority heating in C-Mod**
  – Synthetic diagnostic signal in steady state agrees well with experimental measurements



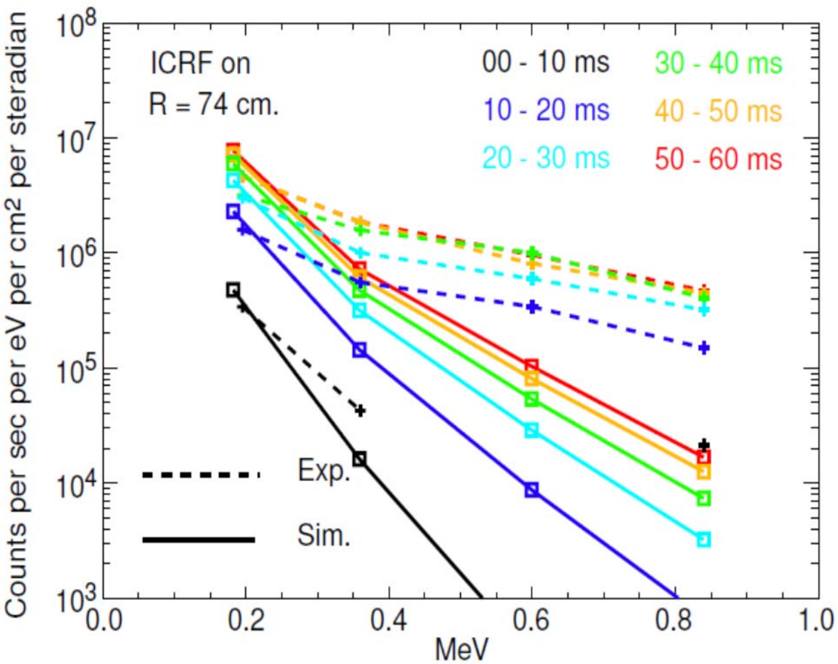
Bader, NF, 2012; MIT PhD Thesis, NS&E, 2011

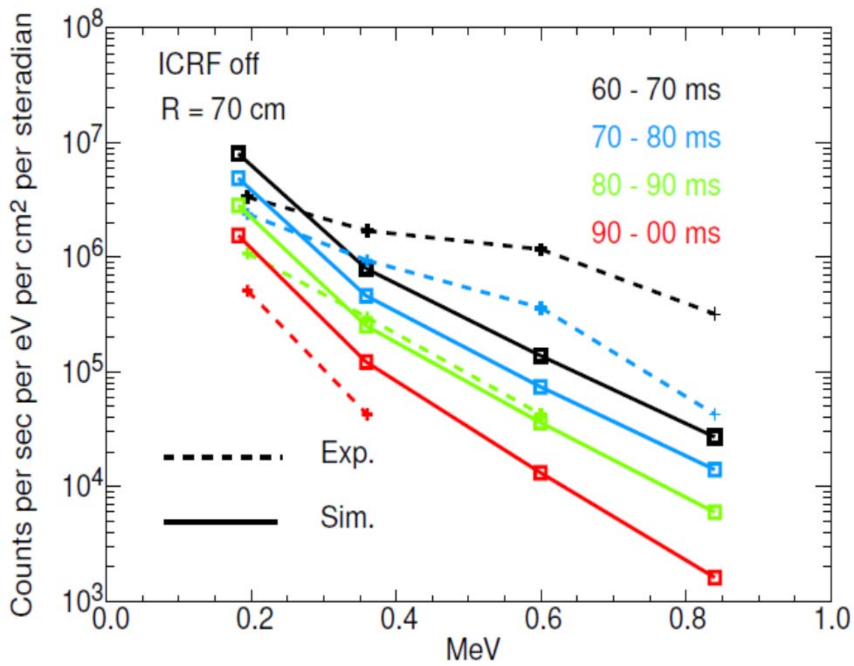
- **Full-wave ICRF fields simulated by the AORSA EM field solver.**



Time dependence of ICRF-generated tail cannot be simulated accurately

- **Simulated CNPA signal lags experimental signal – significantly during tail formation**
- **Decay of simulated CNPA signal is faster than what is measured in experiment during tail decay**





Bader, MIT PhD Thesis, NS&E, 2011

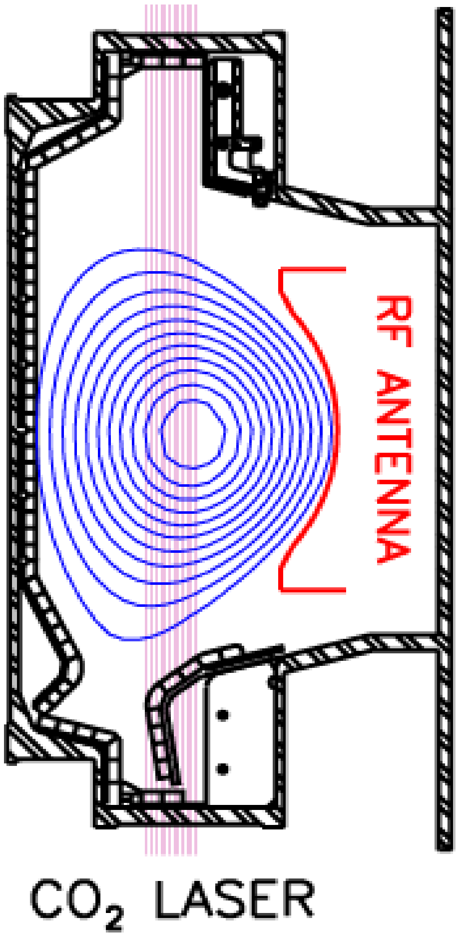
Possible reasons for failure to simulate time dependence of minority ion tail

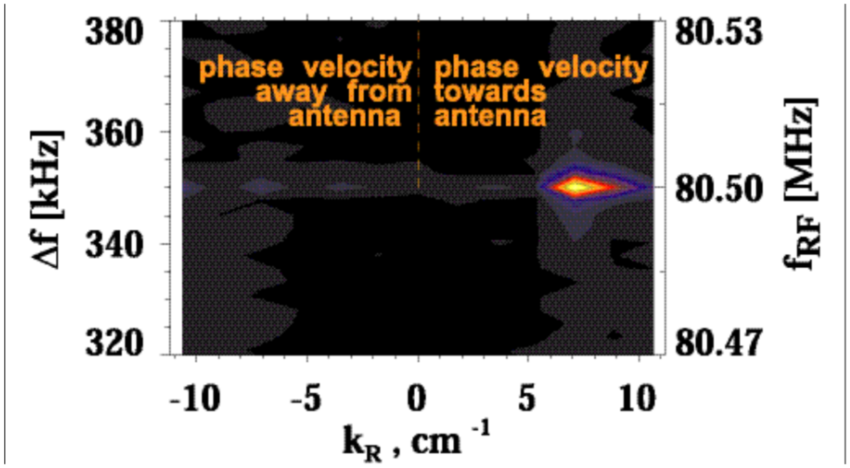
- **Resonant ion may be receiving non-diffusive "kicks" in energy from the ICRF wave:**
  - Coupling between wave solver and Fokker Planck code relies on quasilinear or "diffusive" interaction where successive "kicks" received by the ion from the wave are assumed to be uncorrelated
  - If energy kicks are correlated then formation time of tail would be faster than what is predicted based on quasilinear treatment
  - Does not necessarily explain why the simulated tail decays faster than it does in experiment
- **Finite ion orbit (FOW) width effects may also be important:**
  - Particle-cyclotron resonances and strong quasilinear diffusion occur in roughly vertical planes in zero-orbit width description
  - But orbit topology can move particles away from (or towards) resonances that would be sampled (not sampled) in full-wave solver
- **Simulation approach for treating both these effects has been developed – the "DC" code [Harvey & Petrov, IAEA (2012)]:**
  - Directly integrate the ion orbits using electric fields from a full-wave solver
  - Compute averages of the changes in velocity, pitch angle, and radial position over a complete bounce orbit, to obtain a set of RF induced diffusion coefficients.

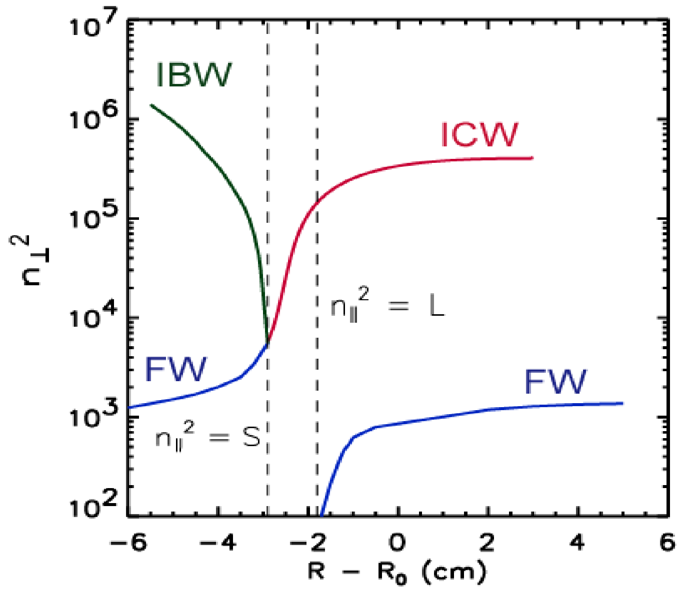
Understanding the mode conversion aspect of ICRF heating has required theory, experiment, and computation

- **Initial observations of mode converted ICRF waves in Alcator C-Mod presented a scientific conundrum:**
- Waves were detected on the tokamak low field side (LFS) and at $k_R \approx 7\ cm^{-1}$
- This was the "wrong" location and wavenumber to be the anticipated ion Bernstein wave (IBW)
- But high resolution full-wave simulations (TORIC and AORSA) also revealed the presence of these waves at the "wrong" location and wavenumber.
- **Mode converted waves are potentially useful for driving poloidal flows that can be used for localized control of the pressure profile.**

Experimental Observation of a "new" type of mode conversion- the ion cyclotron wave (ICW) – a cold plasma electromagnetic mode

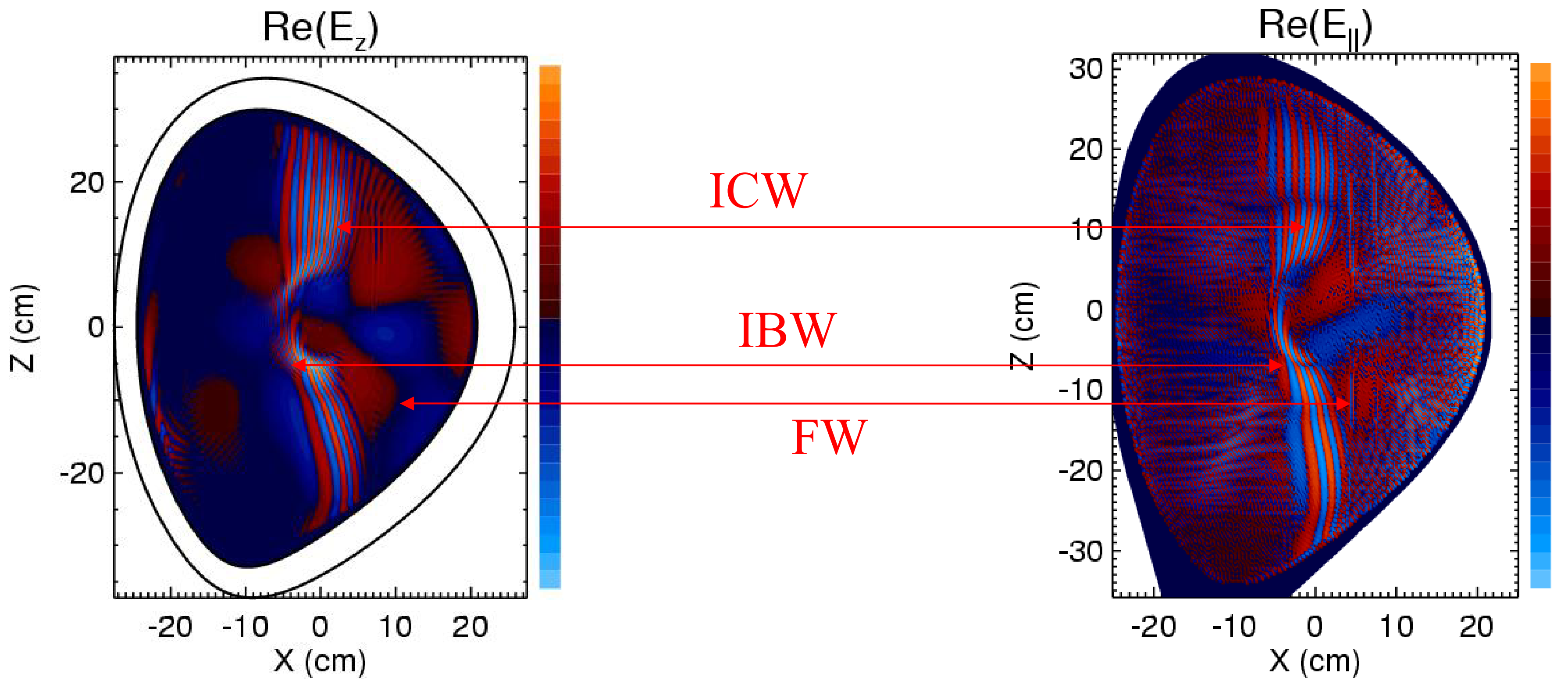






A. Mazurenko, PhD thesis, MIT (2001).
Nelson-Melby et al, PRL 90 (2003) 155004

Both the TORIC and AORSA Solvers also predicted the ICW wave field feature



TORIC at 240N_r x 255 N_m

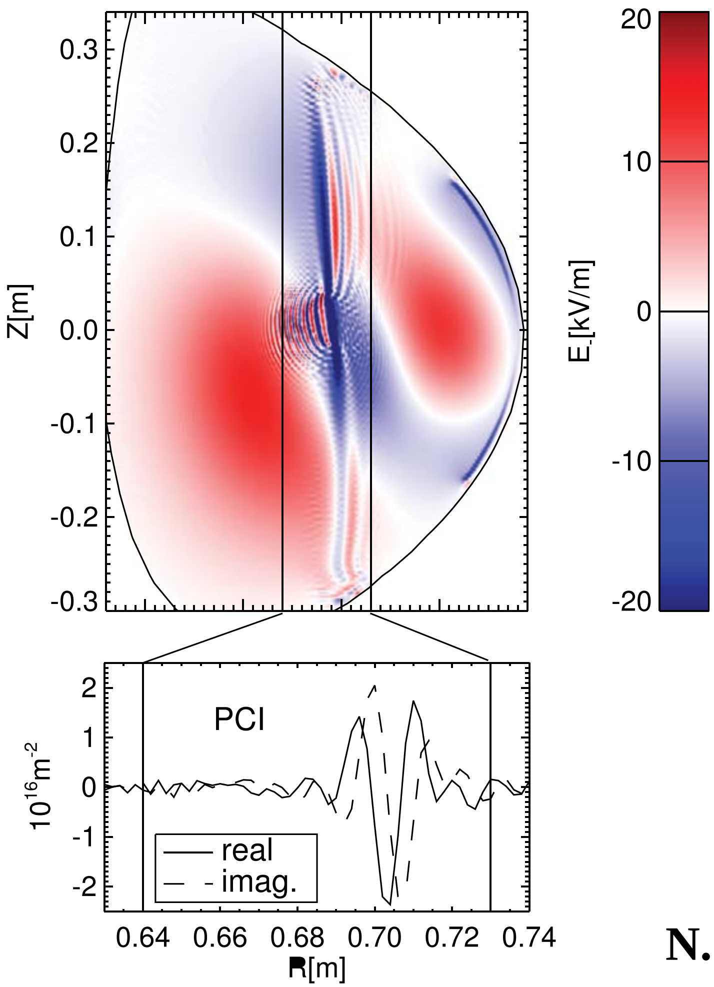
AORSA at 230N_x x 230 N_y

- **In fact the mode converted ICW had been predicted to exist years ago [F. W. Perkins, Nuclear Fusion (1977)] but had been forgotten.**

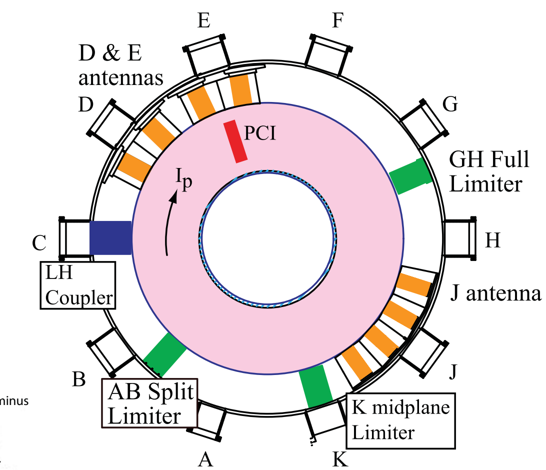
J. C. Wright PoP (2004)

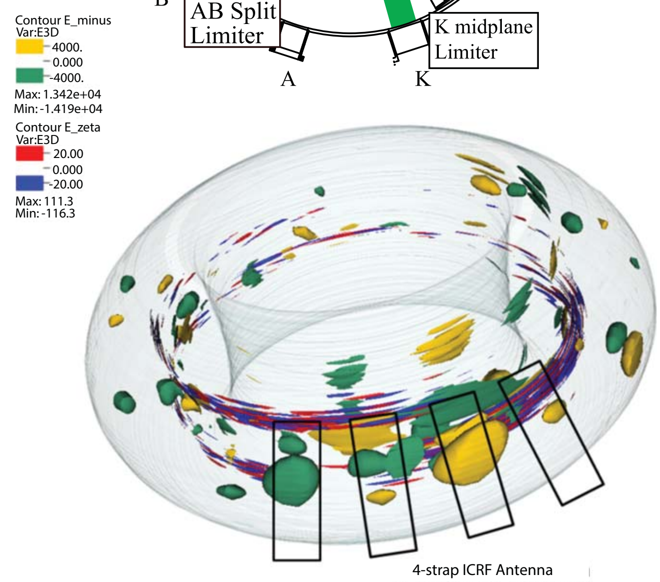
Phase Contrast Imaging (PCI) Diagnostic used to validate the mode conversion physics in the full-wave solvers

AORSA simulation of RF electric field and reconstructed PCI signal for a D(^{3}He) plasma in Alcator C-Mod



- **PCI diagnostic is displaced toroidally from the 'D', 'E', and 'J' ICRF antennas which necessitates 3D ICRF field reconstructions**

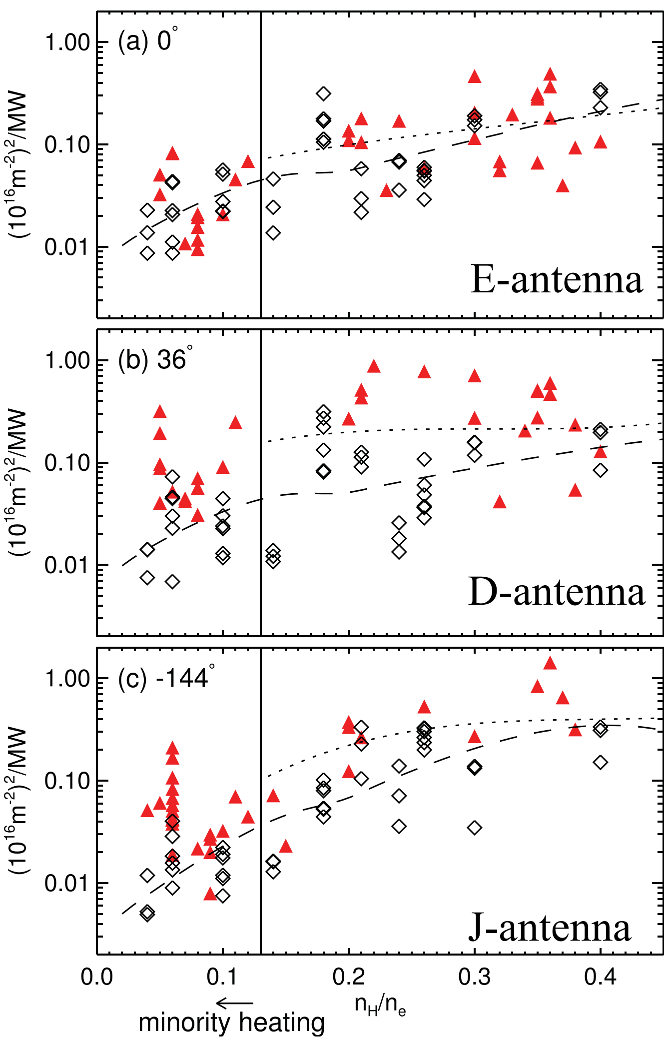


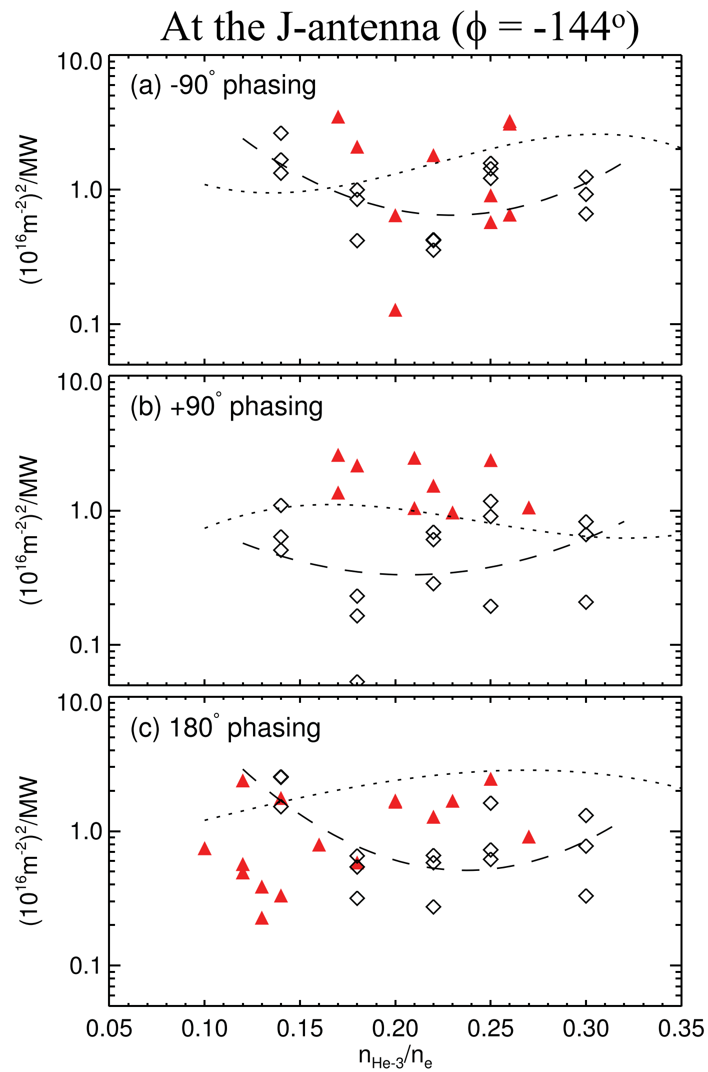


N. Tsujii, PoP (2015)

Simulated and measured PCI signals agree well over a wide range of ‘minority’ hydrogen and Helium-3 concentrations

- **Comparison of the measured (red triangles) and simulated (open triangles) PCI signal intensities for D(H) and D(^{3}He) plasmas in C-Mod**



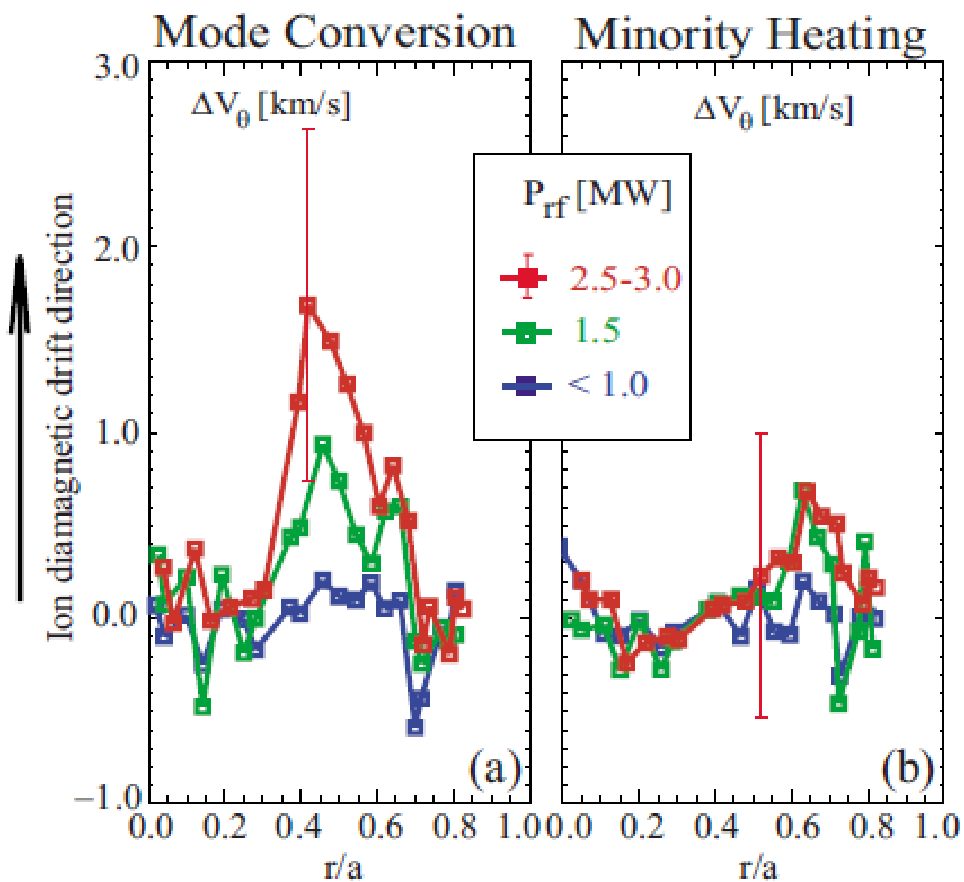


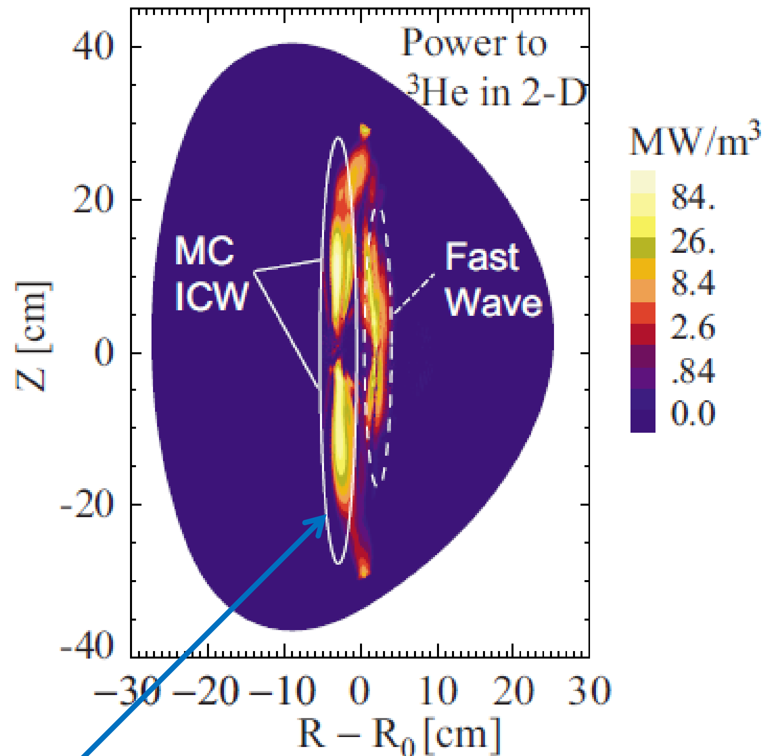
Dashed curves are fits to AORSA points

Dotted curves are fits to TORIC points

N. Tsujii PoP (2015)

Mode converted IBW and ICW were used in C-Mod and TFTR to drive significant poloidal flows [1,2]





[1] Y. Lin *et al*, PoP **16**, 056102 2009.
[2] C. K. Phillips *et al*, NF **40**, 461 2000.

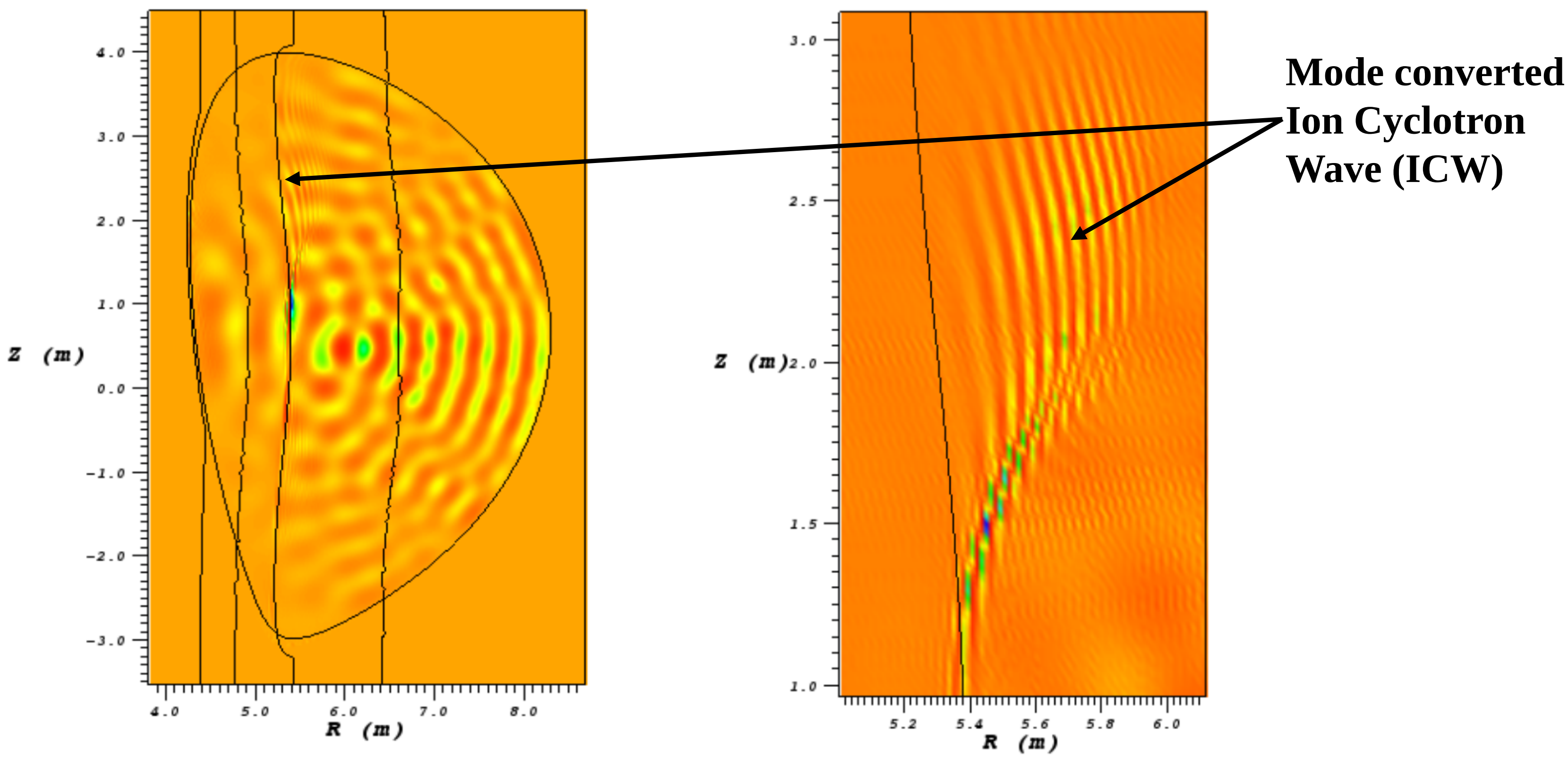
- **ΔV_θ found to scale with P_{rf}**
- **Full-wave analysis [1] indicates strongest flow drive regime associated with ICW damping on ions at ^{3}He resonance**
- **No predictive theoretical / computational formulation yet for flow drive effect**

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, $n = 2.5\text{x}10^{19}$ m^{-3}

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

E_perp **Blowup (E_parallel)**

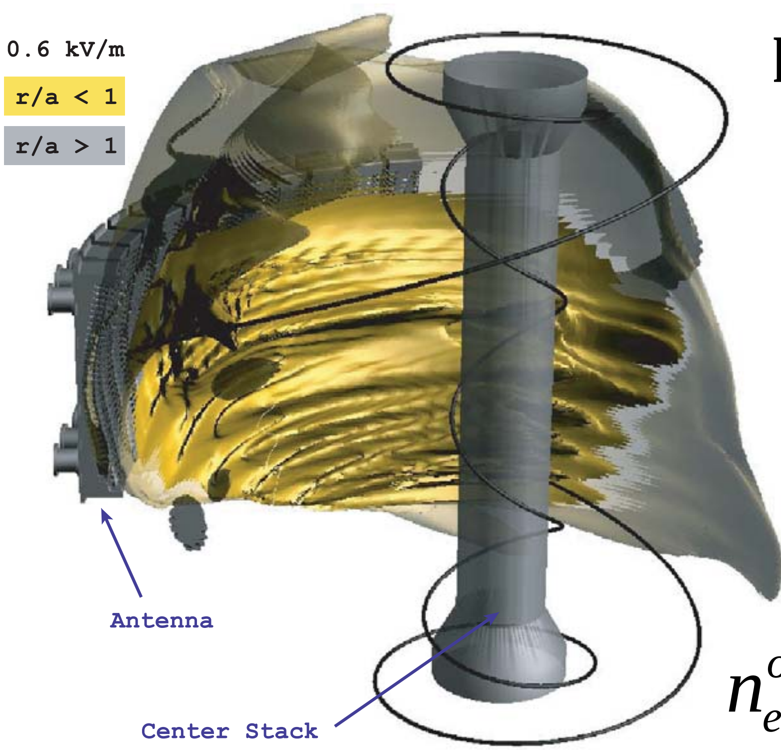


E. F. Jaeger PoP (2008)

Simulation of ICRF antenna coupling and interactions with the SOL and plasma facing components remains a “grand challenge” problem

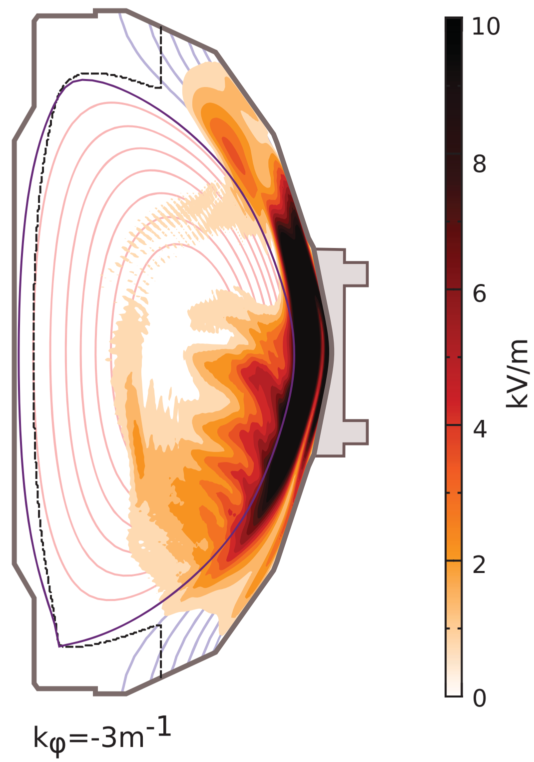
- **Important processes to treat are nonlinear RF sheath formation and surface wave excitation**
- The SOL plasma strongly affects the wave coupling to the core, and the RF fields are expected to modify the SOL
- Both linear and nonlinear interactions must be studied with high fidelity to enable quantitative predictions for present-day devices and ITER
- **Simulation models must couple core and edge:**
  - Spectral solvers are ideally suited for describing ICRF wave physics in the core because the RF plasma response can be formulated in a wavenumber basis set
  - Finite element domain and finite difference codes are best for describing the complicated geometry of the tokamak vacuum vessel and ICRF antenna
  - Core spectral solvers such as AORSA have been extended to the edge
  - Promising approach is combining core spectral codes and finite element domain or finite difference edge codes using admittance matching, mode matching or direct solution matching techniques at the edge

ICRF full-wave solver (AORSA) has been extended to the vessel wall and used to elucidate surface mode excitation during high harmonic fast wave (HHFW) heating in NSTX [Green PoP (2011) & Bertelli NF (2014)]



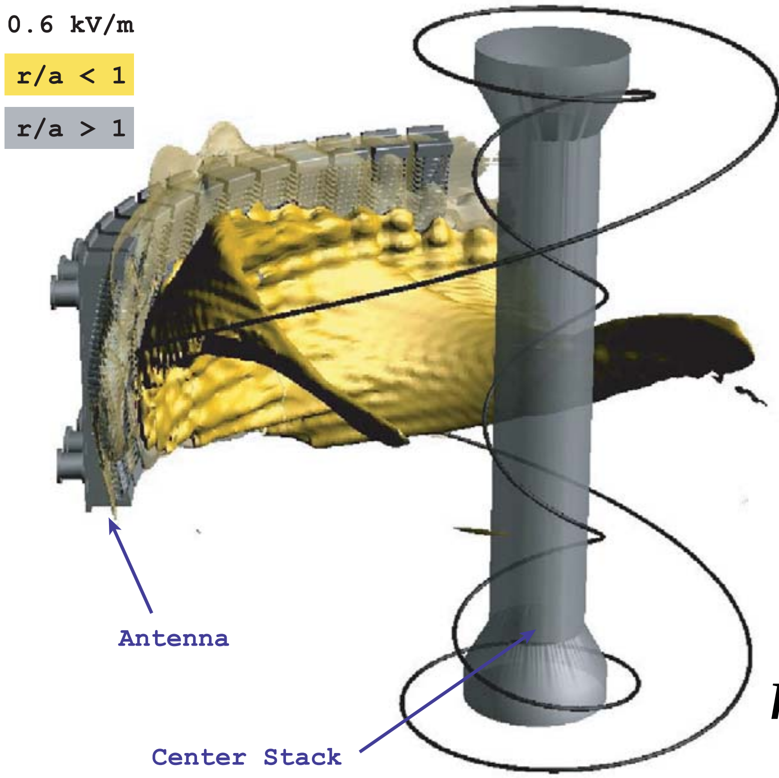
$k_\phi = -3m^{-1}$

$$n_e^{onset} \propto \frac{Bk_\phi^2}{\omega}$$



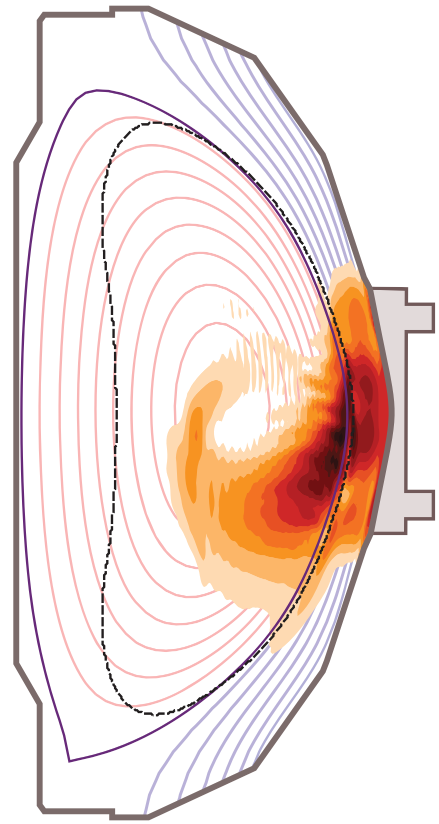
- **Physical interpretation is that at low k_ϕ the onset density for HHFW propagation lies close to the antenna so that a fast wave is excited in the SOL that is confined between the density pedestal at the LCFS and the vessel wall.**

At higher antenna wavenumber ($k_\phi = \pm 13 m^{-1}$) core wave penetration of the HHFW power is recovered in agreement with experimental results on NSTX [Hosea PoP (2008)]



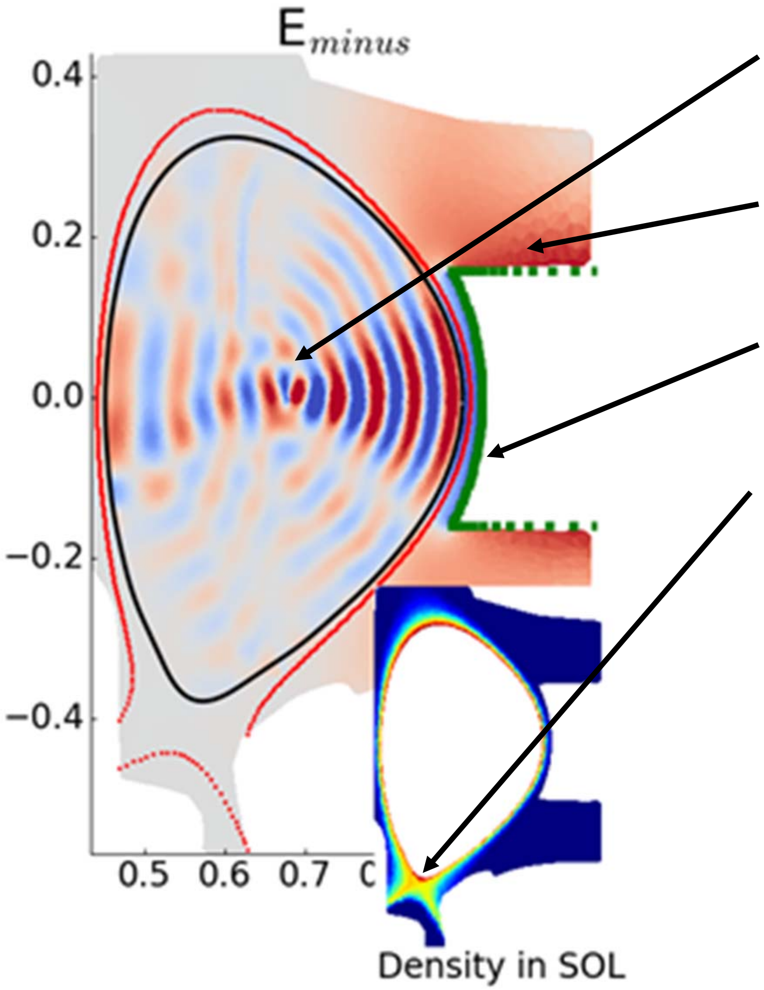
$k_\phi = \pm 13 m^{-1}$

$$n_e^{onset} \propto \frac{B k_\phi^2}{\omega}$$



- At $k_\phi = \pm 13\ m^{-1}$ surface wave excitation is avoided because onset density for wave propagation occurs at higher density which is nearer plasma LCFS.

Initial attempts have been made at combining core spectral solver (TORIC) with an edge finite element domain code (COMSOL)

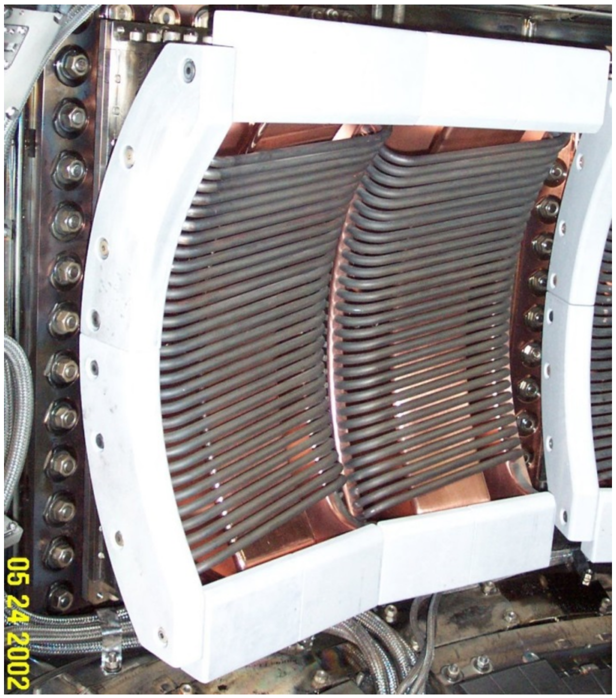


- Core wave propagation is simulated by spectral solver - TORIC
- Cold plasma wave propagation in the SOL is simulated using COMSOL
- ICRF antenna is modeled as a simple current strap with COMSOL
- Realistic SOL density profile and shape in open magnetic field geometry are simulated with COMSOL
- Both core and edge are linear problems so that a solution can be obtained by linear combination of solutions obtained by different boundary values (so-called mode matching technique).

J. C., Wright & S. Shiraiwa RF Conf. (2015)

ICRF launchers in contact with plasma are subject to nonlinear effects, leading to parasitic power posses.

Alcator C-Mod Dipole Antenna



- Electrons are preferentially accelerated out of the region that is contact with plasma creating a thin ion rich layer called a sheath

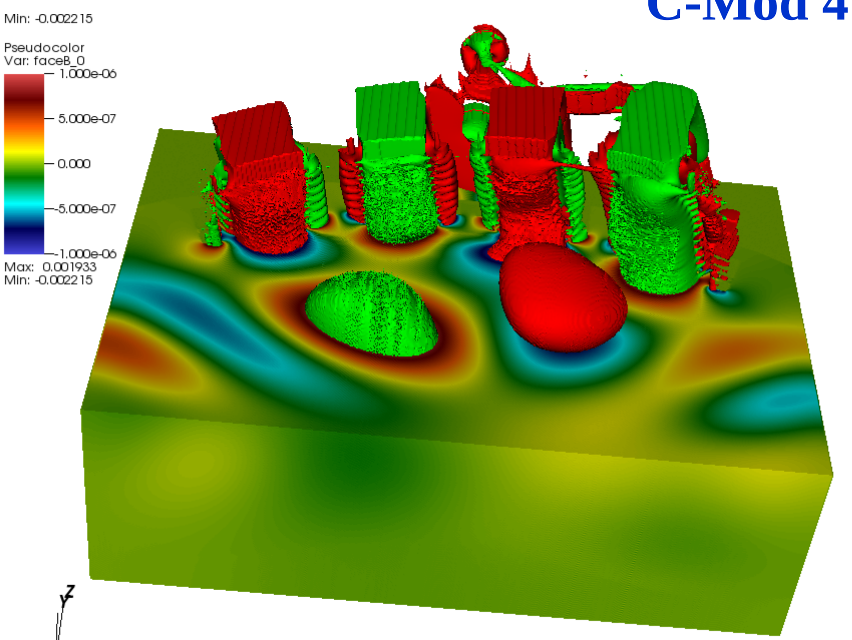
- Voltage (V_{sh}) is set-up to maintain ambipolarity in this region which depends nonlinearly on the sheath width (Δ_{sh}) through the Child-Langmuir Law:

$$\Delta_{sh} \propto V_{sh}^{3/4}$$

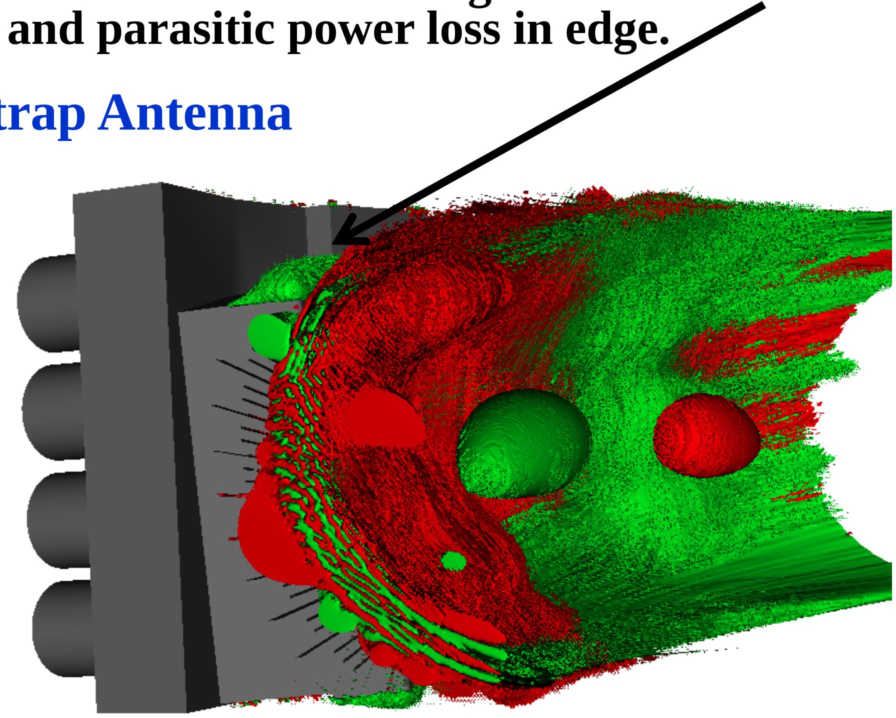
- ICRF antennas typically couple an $E_{//}$ due to a mismatch between equilibrium **B** and the antenna structure.
- This $E_{//}$ excites a slow wave mode in the edge depending on the local density which enhances the sheath voltage to levels > 100 V which can lead to sputtering at metal surfaces and parasitic power losses.

Simulation of ICRF antenna coupling and interactions with plasma facing components remains a "grand challenge" problem

- **Antenna coupling models with nonlinear RF sheaths are being developed to understand and minimize parasitic RF power losses in ITER:**
  - **Realistic 3D geometry, with sheath voltage, to estimate sputtering and impurity production.**
  - **Use of realistic edge density may also lead to understanding of slow wave generation, surface wave excitation and parasitic power loss in edge.**



C-Mod 4 Strap Antenna



Jenkins (2014): 1.3 Billion grid cells, 184,320 cores, 1,000,000 CPU hours on Titan

Summary

- Reviewed the salient physics features of wave propagation, mode conversion, and absorption in the ICRF regime in tokamaks
- Gave examples of how high performance computing (HPC) has advanced our understanding of the following:
  - Generation of energetic ion tails by ICRF power where the effects of modifications of the ion tail distribution are self-consistently included in the wave propagation
  - How long wavelength magnetosonic waves can mode to extremely short wavelength modes such as ion Bernstein waves and ion cyclotron waves
  - How details of the scrape off layer can profoundly impact wave coupling and potentially lead to parasitic losses
  - High physics fidelity in models that is enabled by HPC makes detailed comparisons between measured data and synthetic diagnostics possible
- The computational techniques and physics issues described in these lectures for ICRF wave propagation are often applicable to the higher frequency HHFW regime and the lower hybrid range of frequencies (LHRF)