Status of RF Modeling in Integrated Simulations

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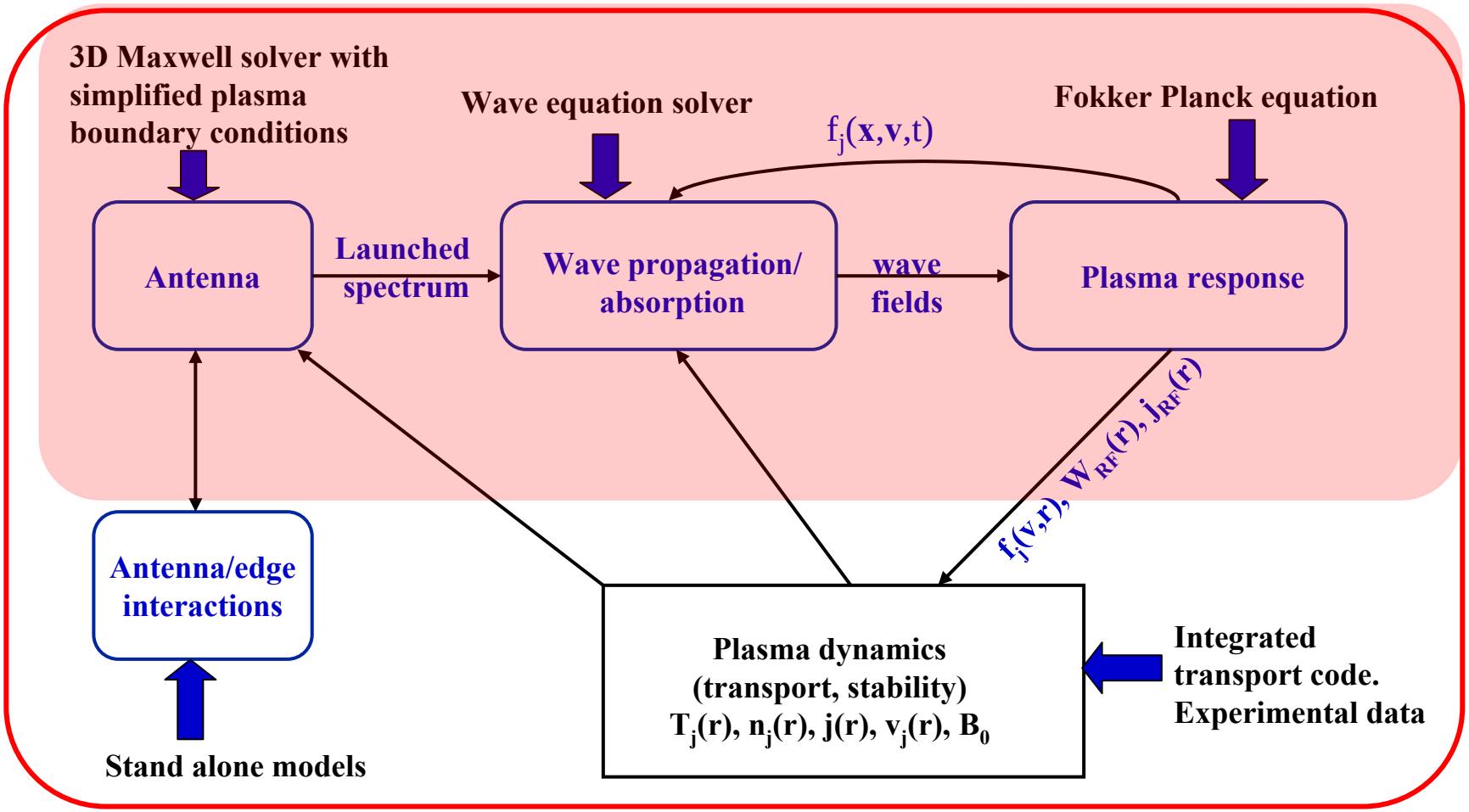
Integrated RF modeling requires a number of interconnected components



Integration

Basic equations of wave propagation and absorption

$$\nabla \times \nabla \times \mathbf{E} + \frac{\omega^2}{c^2}\mathbf{E} = \mathbf{J}_P \circ \mathbf{E} + \mathbf{J}_{ant} \quad : \quad + \text{boundary conditions}$$

plasma wave current: an integral operator on E

- **Time harmonic ↔ real ω, coherent waves, spatial damping**
- **$\mathbf{J}_{ant}$ = antenna source current**
- **Boundary conditions: bounded domain – conducting or inhomogeneous source region**

- **Weakly non-linear, time average distribution function f_0(v, t) evolves slowly:**

$$f(\mathbf{x},\mathbf{v},t) = f_0(\mathbf{x},\mathbf{v},t) + f_1(\mathbf{x},\mathbf{v})e^{-i\omega t}$$

slow, quasilinear time scale ~ τ_E **Fast, RF time scale**

- **$\mathbf{J}_p$ = fluctuating plasma current due to wave – non-local, integral operator on E**

$$\mathbf{J}_P(\mathbf{x},t) = e\int d^3\mathbf{v}\mathbf{v}f_1(\mathbf{x},\mathbf{v},t) \qquad f_1(\mathbf{x},\mathbf{v},t) = -\frac{e}{m}\int_{-\infty}^{t} dt'\mathbf{E}_1\left(\mathbf{x}'(\mathbf{x},\mathbf{v},t'),t'\right)\cdot\frac{\partial f_0}{\partial \mathbf{v}'}$$

- **Approximate operator locally by integrating along guiding center orbits**
- **Effectively uniform plasma conductivity (Stix) →** $\sigma(k_\parallel,k_\perp,\omega) \Rightarrow I_\ell(k_\perp\rho),\ Z\left(\frac{\omega-\ell\Omega_c}{k_\parallel v_{th}}\right)$

Status of ICRF Wave Propagation Codes

- **Full-wave studies of minority heating in 2D are 3D are routine.**

- **Full-wave studies of mode conversion in 2D are now practical.**

- **General (non-Maxwellian) ion distributions from Fokker Planck solvers have been used to formulate the RF conductivity in wave codes, providing for full self consistency.**

- **Larger memory and higher processing capability of massively parallel architectures was largely responsible for these advances:**
  - **Higher resolution led to improved physics understanding**

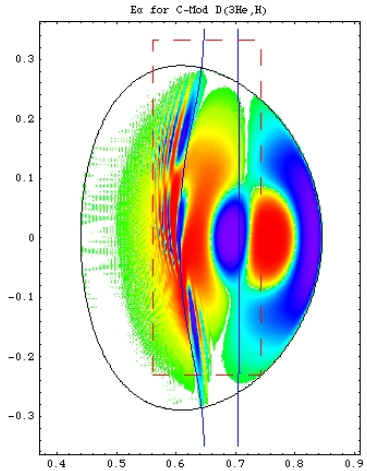
- **Mode conversion in 3D still problematic**

Four full-wave ICRF solvers were advanced within the US SciDac Initiative

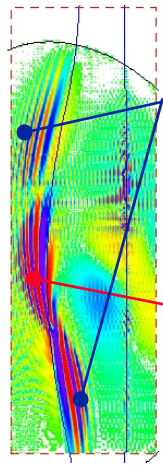
- **All Orders Spectral Algorithm (AORSA) – 1D, 2D & 3D (Jaeger)**
  - Spectral in all 3 dimensions
  - Cartesian/toroidal coordinates (x, y, ϕ)

$$\mathbf{E}(\mathbf{x}) = \sum_{n,m,l} \mathbf{E}_{\mathbf{n,m,l}} e^{i(nx+my+l\phi)}, \quad \sigma \to \sigma(x, y, \phi),$$

  - Includes all cyclotron harmonics
  - No approximation of small particle gyro radius ρ compared to wavelength λ
  - Produces huge, dense, non-symmetric, indefinite, complex matrices



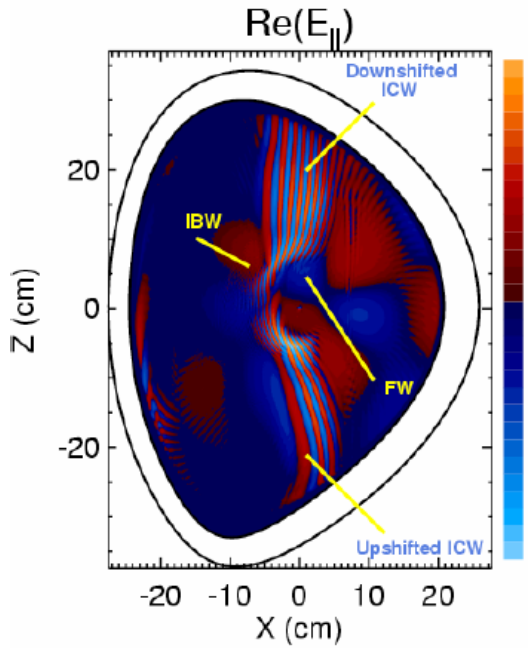
Blowup region



- **TORIC – 2D (Brambilla/Bonoli/Wright)**
  - Mixed spectral (toroidal, poloidal), finite element (radial)
  - Flux coordinates (ρ, θ, ϕ)

$$\mathbf{E}(\rho, \theta, \phi) = \sum \mathbf{E}_{\mathbf{m,l}}(\rho) e^{i(m\theta+l\phi)}, \quad \sigma \to \sigma(\rho, \theta)$$

  - Up 2nd cyclotron harmonic
  - Expanded to 2nd order in ρ/λ
  - Sparse banded matrices

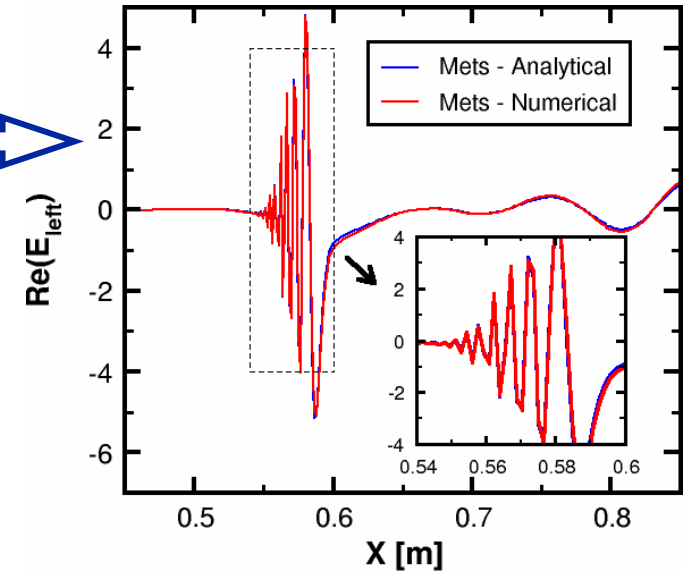


Four full-wave ICRF solvers were advanced within the US SciDac Initiative

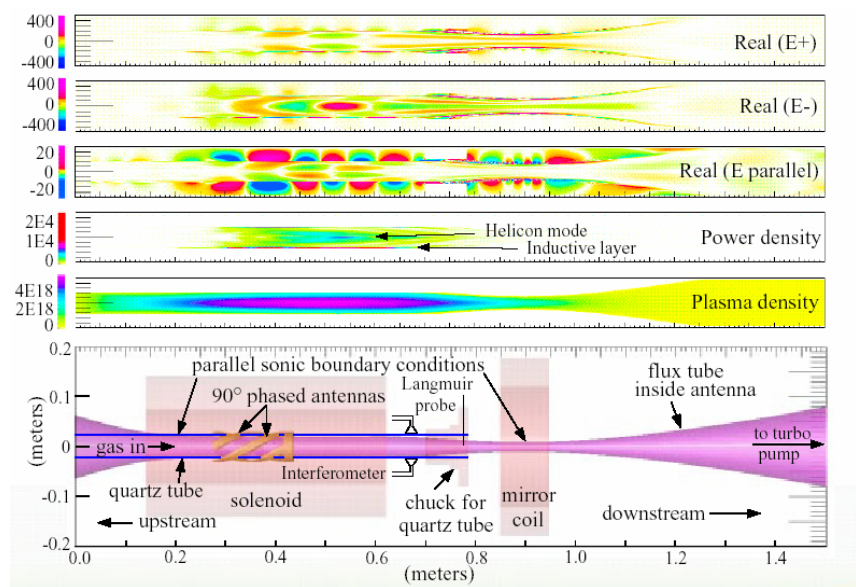
- **METS-1D (D. N. Smithe/Phillips) → All orders, fully spectral code in 1D**

$$\mathbf{E}(\mathbf{x}) = \sum_{n,m,l} \mathbf{E}_{\mathbf{n,m,l}} e^{i(nx+my+l\phi)}, \quad \sigma \rightarrow \sigma(x)$$

  - **Includes all cyclotron harmonics**
  - **No approximation of small particle gyro radius ρ compared to wavelength λ**
  - **Used for benchmarking studies compared to 2D, development platform for non-Maxwellian conductivity operator routines**



- **MORFIC**
  - **Finite difference**
  - **Adapted for open field line systems: plasma propulsion, simplified stellarator geometry**
  - **Iterates with source/transport model**

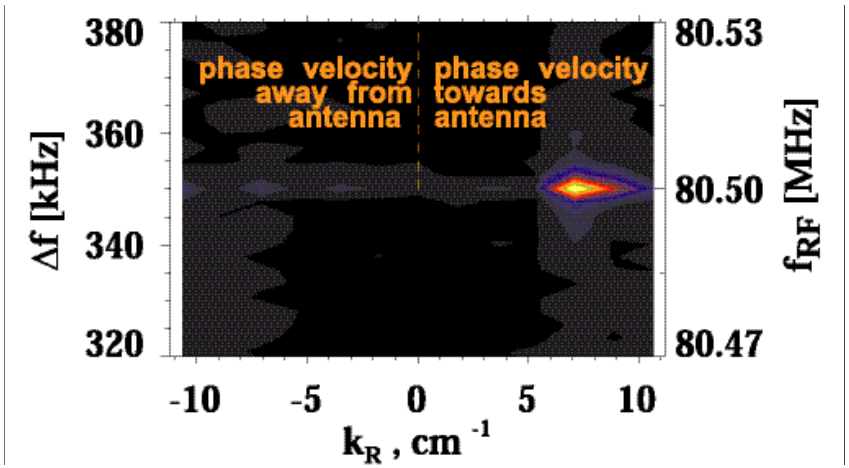


ICRF Mode Conversion Physics in 2D

- **Initial observations of mode converted ICRF waves in Alcator C-Mod presented a scientific conundrum:**
  - **Waves were detected on the tokamak 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 our full-wave simulations (TORIC and AORSA) also revealed the presence of these waves at the "wrong" location and wavenumber.**

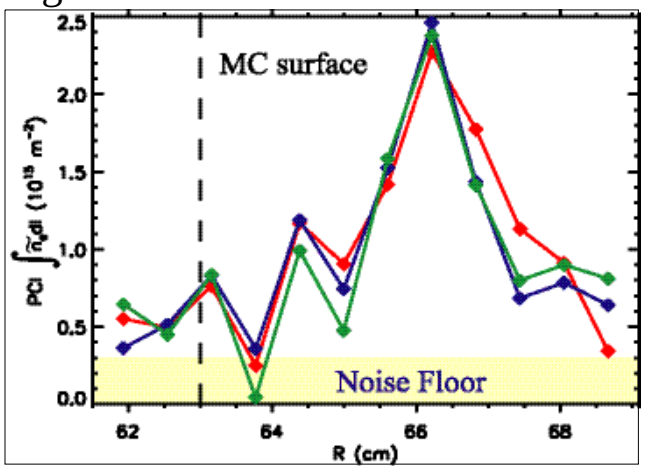
Experimental Observation of ICW*
*[E. Nelson-Melby *et al*, PRL, 90 (15) 155004 (2003)]

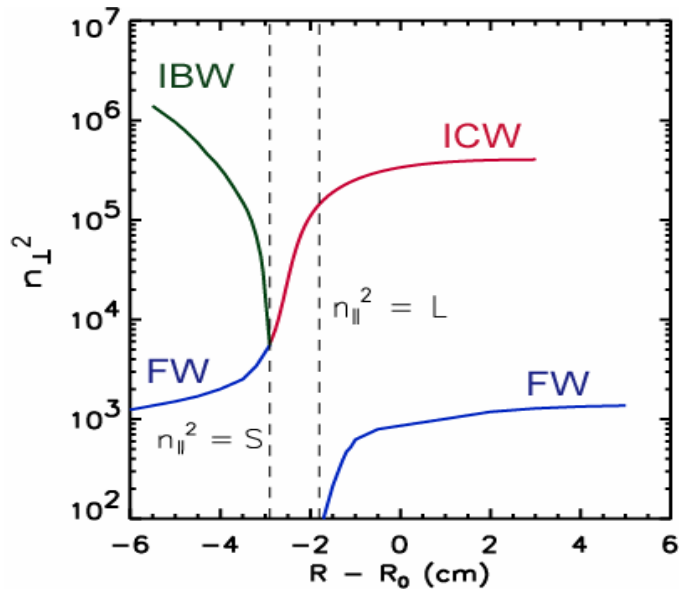
Contour Plot of Fourier Analyzed PCI Data



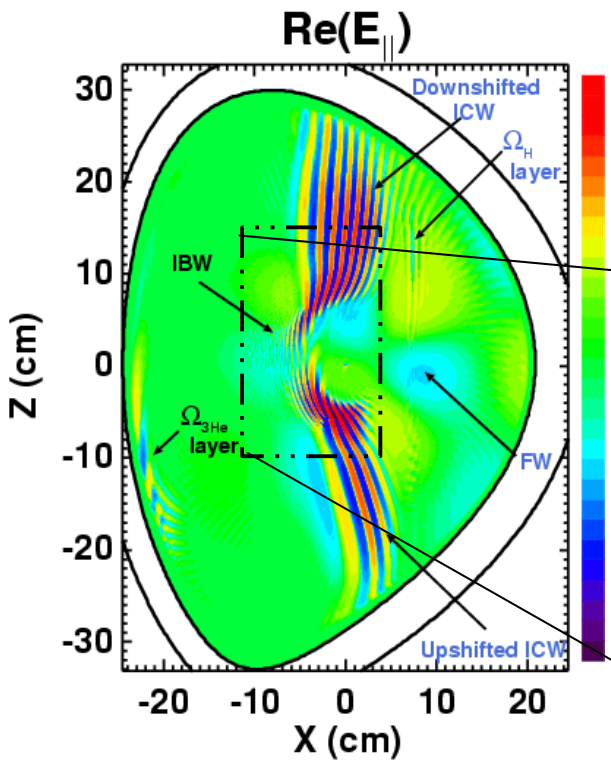
- **Detected wave propagates towards the low field side.**
- **Wavelength shorter than FW, but generally longer than IBW.**
- **Signal is located on the low field side of the H-^{3}He hybrid layer.**

PCI Signal Structure

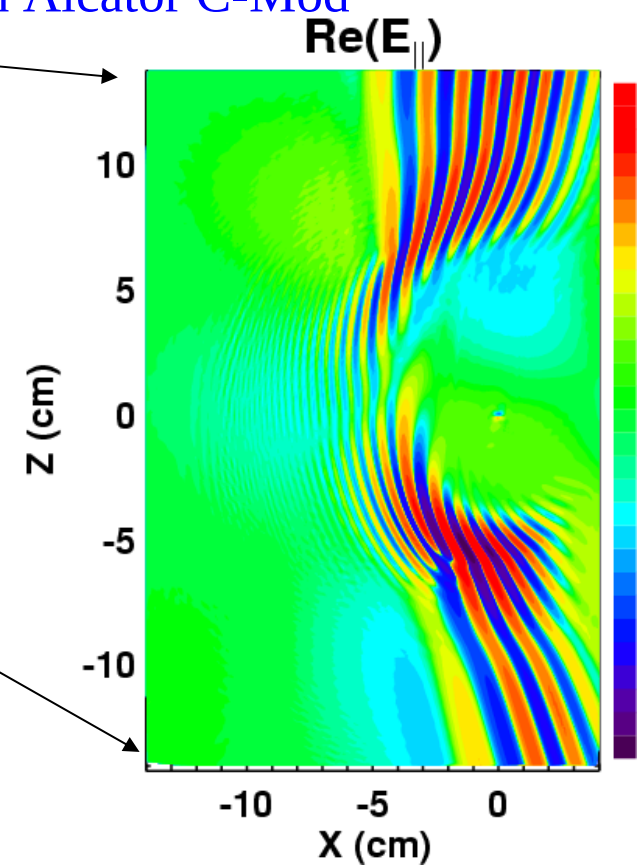




2D ICRF Mode Conversion Physics



- Three waves – IBW, ICW, FW – are resolved at the MC layer.
- The 2-3 wavelengths of IBW seen in simulations have been verified by PCI measurements on Alcator C-Mod



- The intermediate wavelength ICW travel towards the low field side above and below the midplane.
- Poloidal field allows coupling to ICW (Perkins 1977)

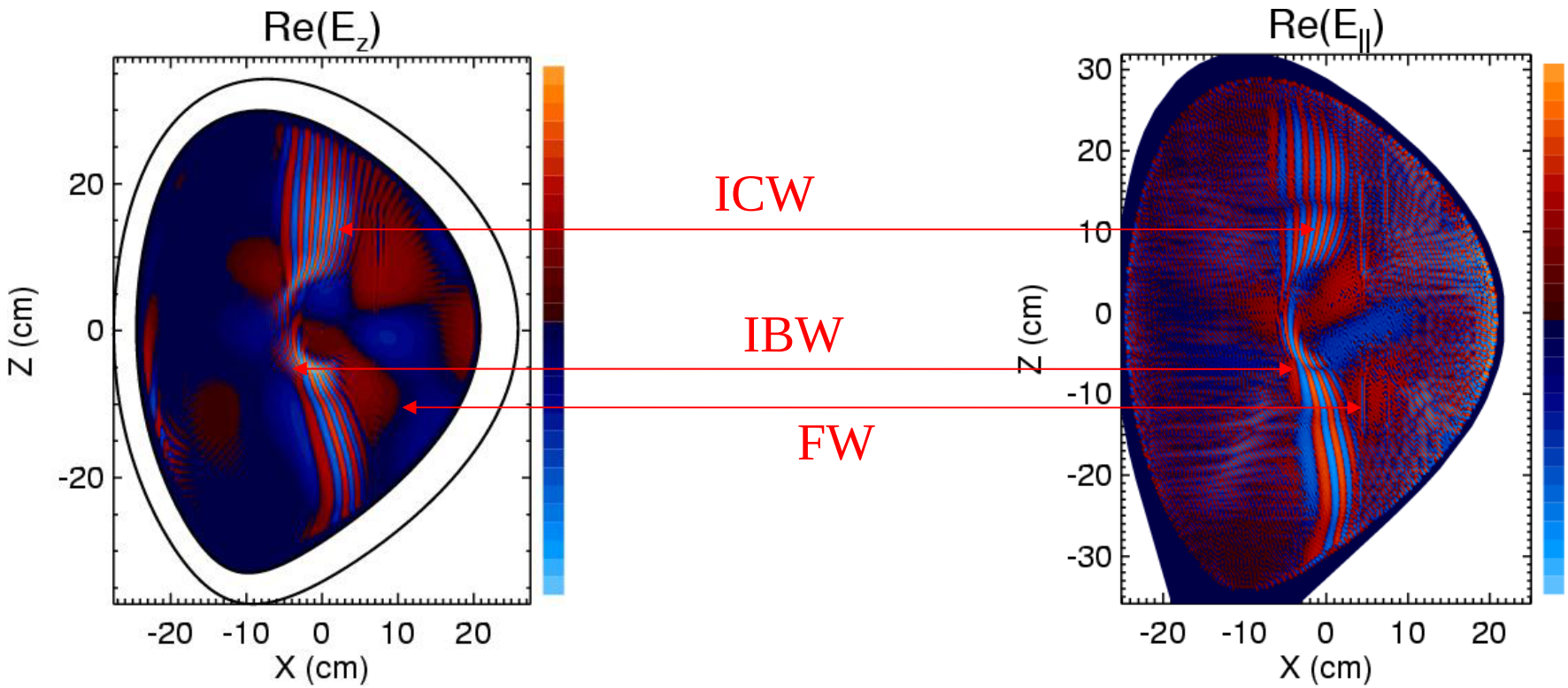
Role of B_p in the Mode Conversion Process

- **Presence of $B_p(\psi)$ allows coupling of the fast wave to an ion cyclotron wave (ICW) [F.W. Perkins, 1977] - a 2D effect !**
- Mode converted waves are characterized by relatively large m $\Rightarrow$ [$|m| > 100$]:

$$k_{//} = \frac{m}{r}\frac{B_\theta}{B} + \frac{n}{R}\frac{B_\phi}{B}$$

- **ICW propagating back to the LFS have very different $k_{//}$ values above and below the tokamak midplane:**
  - Above: **Low $k_{//}$ allows ICW to propagate farther before damping**
  - Below: **High $k_{//}$ causes ICW to damp rapidly**

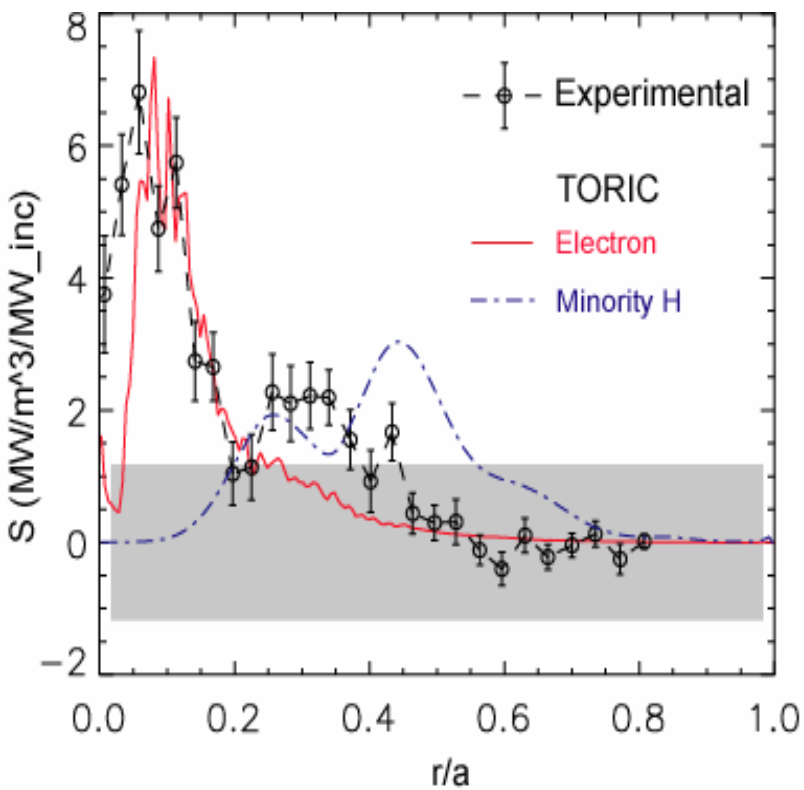
Comparison of TORIC and AORSA - Mode Converted Wave Fields are Similar



TORIC at 240N_r x 255 N_m **AORSA at 230N_x x 230 N_y**

- **Both codes are using the same equilibrium from an Alcator C-Mod discharge with mixture of D-^{3}He-H in (21%-23%-33%) of n_e proportion.**

On-axis Mode Conversion in Alcator C-Mod: D(H)

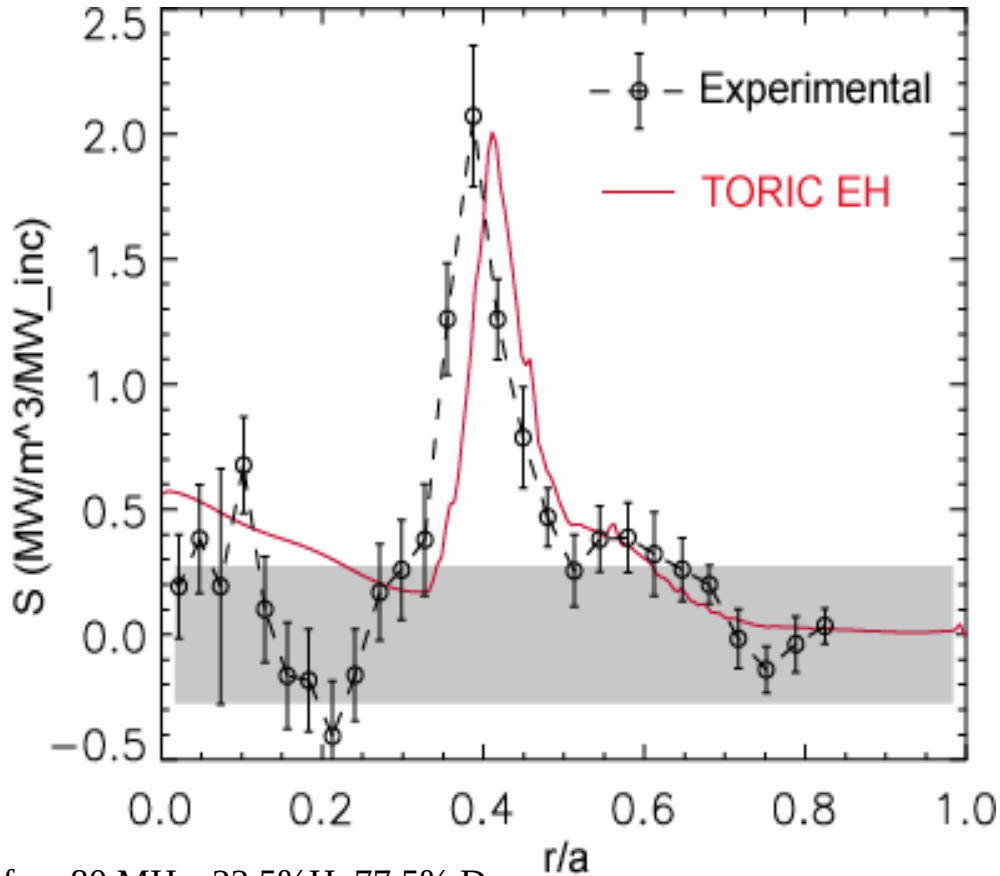


- **Experimental curve agrees with the TORIC simulation in the MC region 0 < r/a < 0.25.**
- **Total volume integrated MCEH power fraction η^{MCEH} :**
  - **Experiment: η^{MCEH} = 16%**
  - **TORIC: η^{MCEH} = 14%**
- **TORIC result also shows IBW is the primary MC wave for this on-axis MC.**
- **B_{pol}, crucial for the existence of MC ICW, is small near axis.**

f_{rf} = 70 MHz, 19%H, 81% D
B_t = 5.27 T, I_p = 1 MA,
$n_e = 1.7 \times 10^{20}\ m^{-3}$, T_e = 1.8 keV
t = 0.8744 sec. J antenna

Y. Lin *et al*: PPCF (2004).

Off-axis Mode Conversion in Alcator C-Mod: D(H)



f_{rf} = 80 MHz, 22.5%H, 77.5% D
B_t = 5.27 T, I_p = 1 MA,
$n_e = 1.8 \times 10^{20}\ m^{-3}$, T_e = 1.8 keV
t = 1.502 sec, E antenna

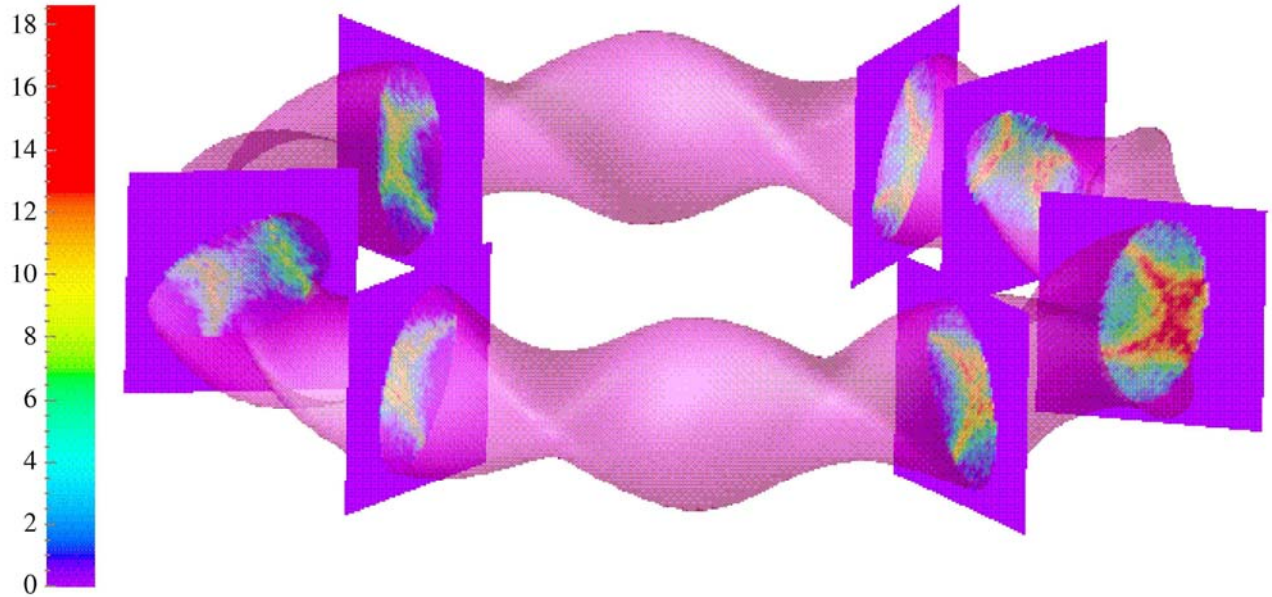
- **Off-axis MC**
  - **D-H hybrid layer at r/a = 0.35 (HFS)**
- **Good agreement of experiment curve and TORIC.**
- **Total η^{MCEH} in the MC region (0.35 < r/a < 0.7)**
  - **Experiment: 20%**
  - **TORIC: 18%**

Y. Lin *et al*: PPCF (2004)

All orders spectral technique has been extended to minority heating in 3D –AORSA3D

- **Preliminary calculation for Fast Wave minority heating on LHD stellarator – 5% minority H in ^{4}He**
- **16× 50×50 modes in ϕ, x, y (10 independent solutions - one per field period, technique of H. Weitzner)**

Fast wave heating in LHD Stellarator



- **Gigantic, dense linear system → NERSC Seaborg, 1600 processor IBM SP, 8 hr processor time at ~1.7 teraflops, memory = 750Mb/processor = 1,200 Gbytes**
- **Convergence study with 32 toroidal modes requires almost 10^6 NERSC MPP**

Status of LHRF Wave Propagation Codes

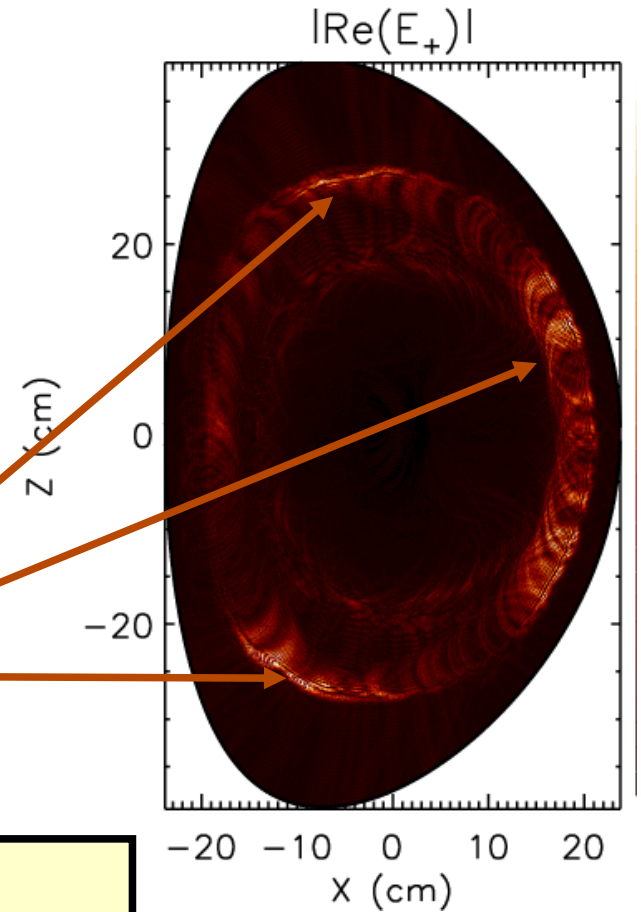
- **Ray tracing in 2D and 3D still the preferred method**
  - **ACCOME, LSC, FRTC, CURRAY, etc**

- **Full-wave studies are now elucidating important physics effects (focusing and diffraction) not easily included in geometrical optics treatments [e.g., Pereverzev, NF (1992)].**

- **Full-wave studies possible through major rewrite of TORIC solver:**
  - **Formulation of the rf conductivity operator in the LHRF**
  - **New boundary conditions at plasma wall to impress $E_{//}$**
  - **Massive parallelization of field solver achieves converged solutions with 1000 radial elements and 1023 poloidal modes.**

FW is transformed to a slow LH Wave at Confluence

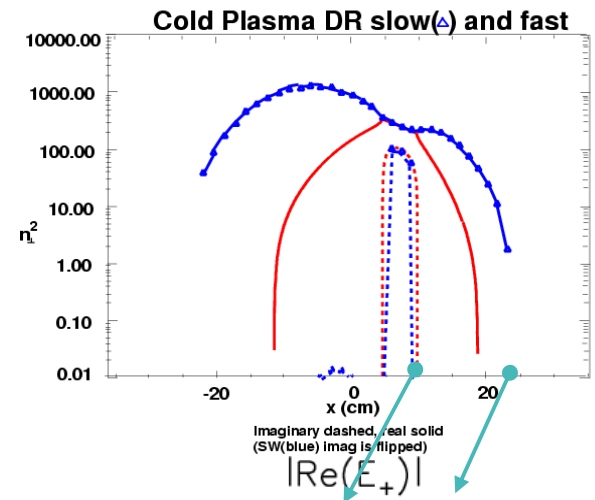
- **At** 4.6 GHz**, a FW polarization is launched from the low field side.** ($n_{||}$=1.5, n_{acc}=2)
- **It is propagative at** X=19 **cm, and undergoes mode transformation to slow LH wave at** X=15 **cm**
- **Loci of LH reflections can be seen in the full wave field patterns - forming caustics.**

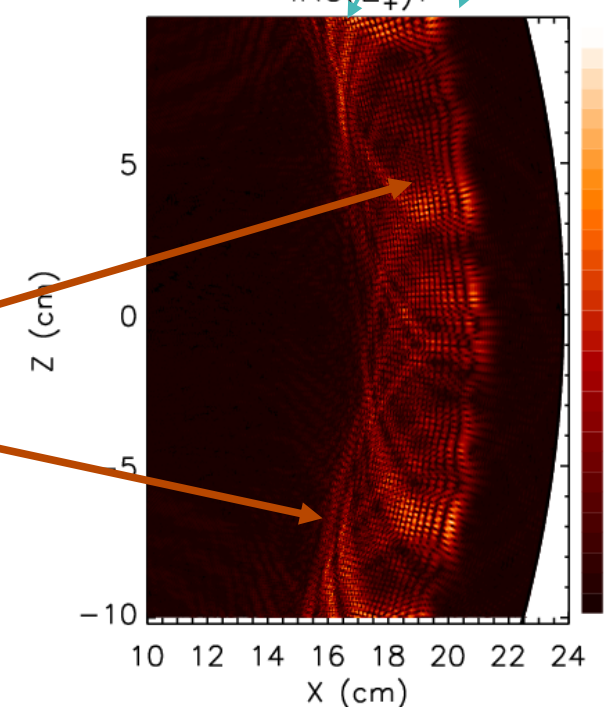


Plasma Parameters:
D(5% H), $n_{||}$=1.5, f=4.6 GHz
B_0 = 5.3 T, T_e=3.5 keV, T_i=2.0 keV
$n_e(0)=1.5\times10^{20}$ m^{-3}, I=1 MA
Nm=1023, Nr=960

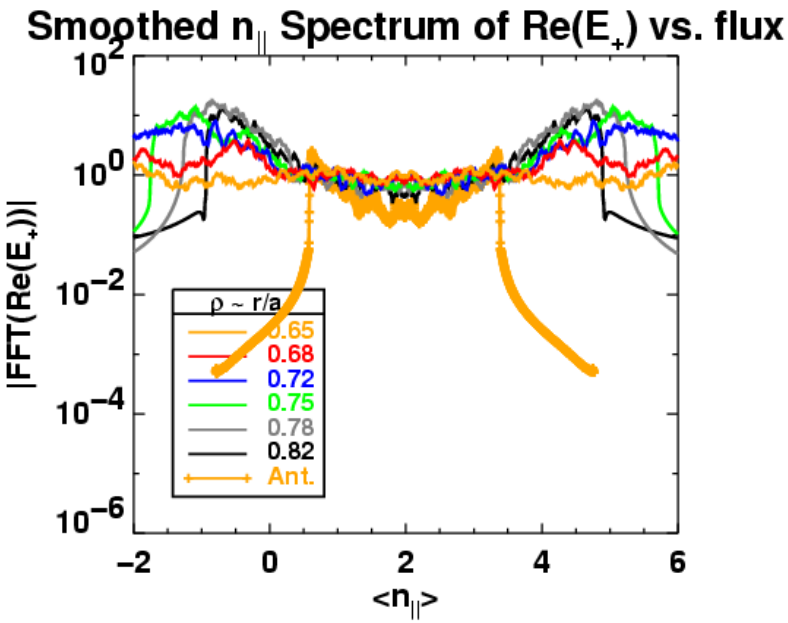
DR describes "Ring" of LH Waves

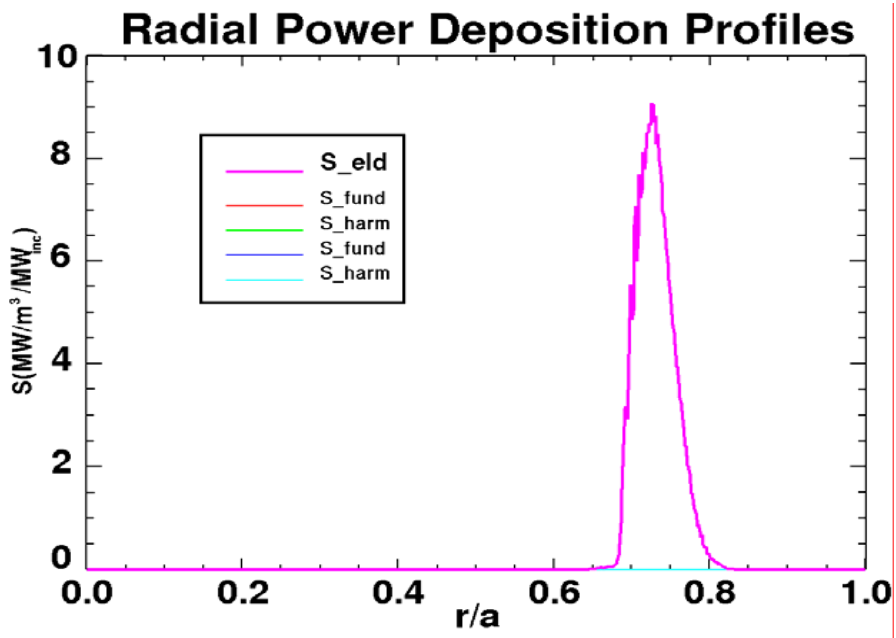
- The FW is coupled at the edge, then mode converts to a slow wave at the confluence.
- The slow wave propagates out to the edge cutoff and reflects inward again to the confluence.
- All wave power is absorbed on the electrons by Landau damping.
- There is a suggestion of resonance cones in the full wave field patterns.
- Caustic formation is also apparent.





Spectral shift is large at caustic





- **The distribution of $n_{||}$ on flux surfaces shows a significant upshift from an averaged launched $n_{||}$ of 2 to >4 in the middle of the annulus at r/a=0.75.**
- **This rapid upshift at the caustic causes all the power to be absorbed in the narrow region bound by the caustic and the edge cutoff - an effect not predicted in geometrical optics !**

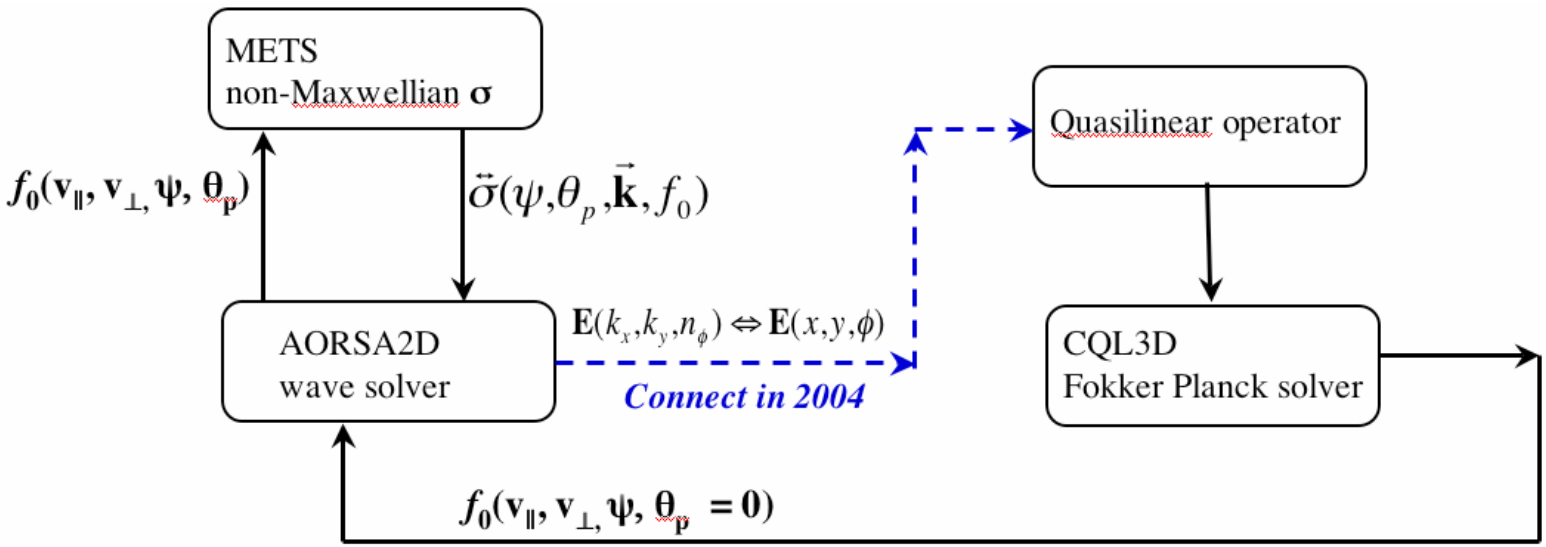
Self-consistency: All the results shown so far assume that f_0 is Maxwellian

- **High power waves can drive the distribution far from Maxwellian**
- **Significant non-Maxwellian components can be produced by neutral injection or fusion alpha particles**

Non-Maxwellian distributions can:

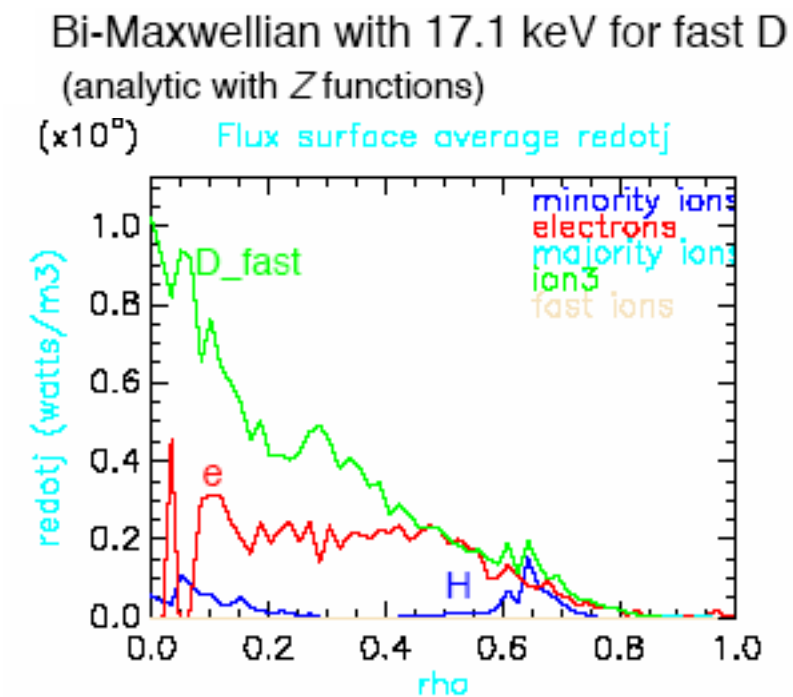
- **Affect local damping rate and wavelength**
- **Modify heating and current drive profiles**
- **Change partition of power deposition among plasma species**
- **Affect mode-conversion**

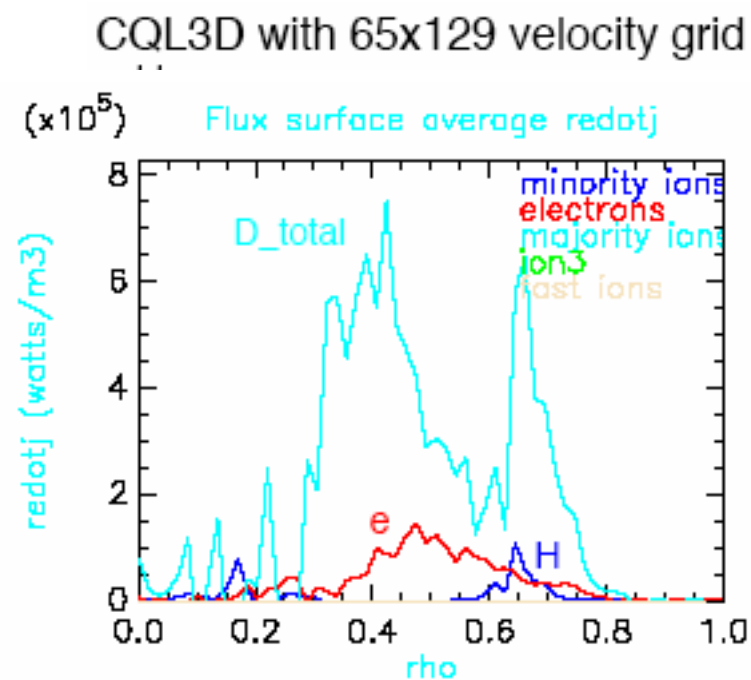
Calculation of wave fields self-consistently with the plasma distribution requires closed loop coupling of four significant physics models



We have obtained results from AORSA2D with numerical distribution functions

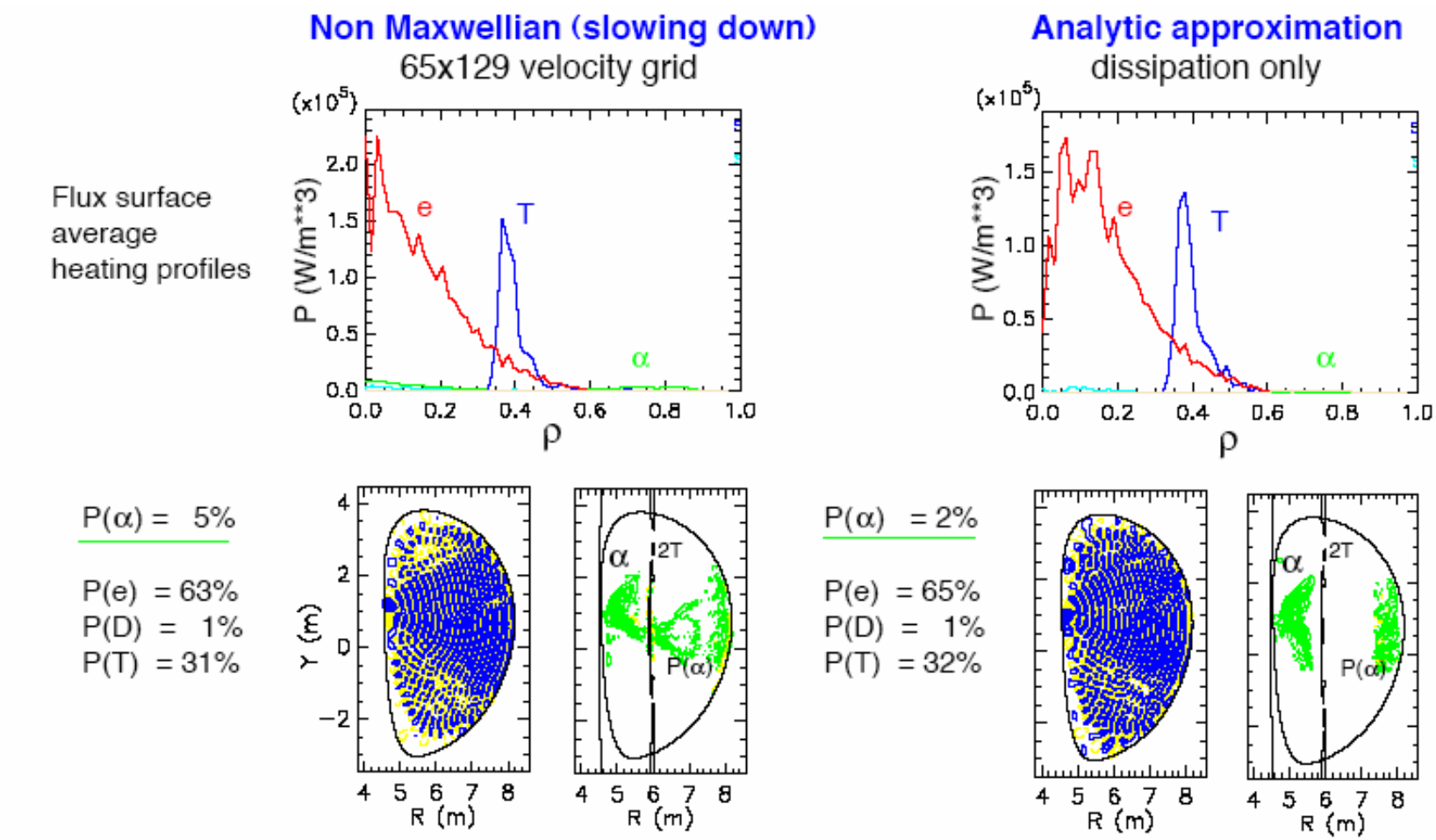
HHFW heating on NSTX with D beam injection:
Comparison of CQL3D distribution with 2 temperature Maxwellian model





- **We see significant differences compared to two temperature Maxwellian model:**
  - **Much narrower ion absorption zones around high harmonic cyclotron resonances**
  - **Much less deposition into electrons: 15%/41%, more power into D: 81%/52%**
- **Non-Maxwellian presently requires about 13× more CPU time – but have already speeded up by 25× and we expect to close the gap**

First converged 2D full wave solutions for ITER scale device, with non-Maxwellian distribution



- **Calculations confirm that fast alpha absorption can be held to low levels with appropriate choice of frequency**
- **Fast alpha population does effect anti-Hermitian part of conductivity enough to modify wave propagation**

Status of Closed Loop Computations of LHCD

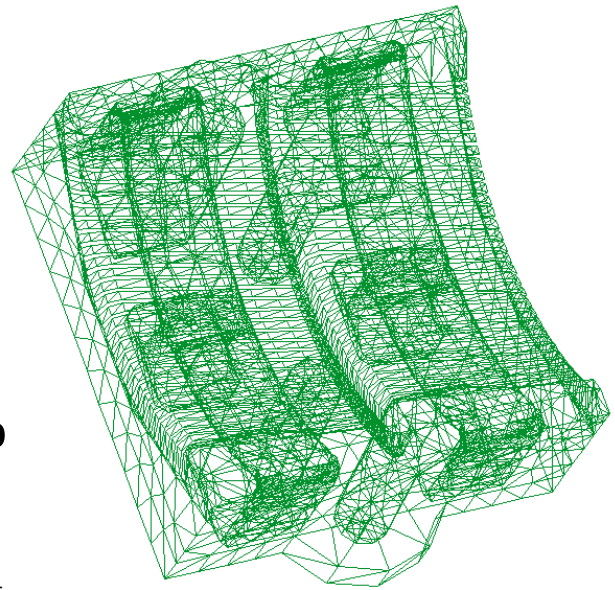
- **Combined Ray tracing plus adjoint methods are still widely used:**
  - **ACCOME, LSC, FRTC, CURRAY, etc**

- **Recent benchmarking studies (Snowmass and ITPA) have shown that exact 2-D Fokker Planck and ray tracing calculations actually predict higher LH currents than adjoint methods:**
  - **CQL3D + GENRAY (US)**
  - **DELPHINE (EU)**
  - **Discrepancy is due to approximate nature of wave induced flux needed with adjoint approach**

- **Implementation of 2D Fokker Planck packages with ray tracing is a natural candidate for parallel platforms:**
  - **Distribute Fokker Planck solution for each flux surface over a separate processor.**
  - **Distribute integration of each ray over a separate processor.**

Coupling to realistic antenna models: TORIC and TOPICA

- First step – done:
  - Set E-field boundary conditions at last flux surface in TORIC
  - Transform TOPICA basis functions into the TORIC space
- Second step:
  - Export Z matrix calculated at LFS in TORIC to TOPICA
  - Calculate reaction integrals needed in TOPICA



CAD rendering of C-Mod antenna used in TOPICA

- The coupling model assumes a coherent plasma antenna surface for this initial phase.
- This collaboration will permit realistic antenna models for both ICRF and LH full-wave studies.

Integration with transport or stability models requires calculation of "macroscopic" plasma response rather than details of f_0

- **Calculation of local power deposition $P_{loc}(x)$, RF driven current, RF macroscopic force to drive fluid flows, or construction of the Quasi-linear operator, involve bilinear functions of the wave field amplitudes**
- **Example: when the plasma response is non-local the power deposition P(x) is not the standard local WKB result**

$$\mathbf{P}_{\mathbf{loc}}(\mathbf{x}) = \tfrac{1}{2}\mathrm{Re}\{\mathbf{J}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x})\}$$

- **P_{loc} is neither symmetric nor positive definite unless:**
  - **σ is independent of k (i.e. local) or**
  - **Only one mode is present (zero spectral width)**
- **In general (finite spectral width) P(x) is a nested double sum over spectrum E_n**

$$\mathrm{P}(\mathbf{x}) = \tfrac{1}{2}\mathrm{Re}\left\{\sum_{m,n} e^{i(k_n - k_m)\cdot \mathbf{x}} \mathbf{W}(k_n, k_m)\mathbf{E}_n \mathbf{E}_m^*\right\}$$

- **In 2D this is 6 nested sums (9 sums in 3D) – not computationally feasible in this form**
- **To evaluate these macroscopic responses we have developed a technique transforming the field spectrum to back to real space, then evaluating a local windowed Fourier transform with fewer modes than the full spectral solution**
- **Speedup of 2000× in AORSA2D with 80 × 80 mode solution**

Optimization is particularly crucial for fully-spectral codes that require solution of large, dense matrices

AORSA codes

- Code restructuring and optimization leads to 50X speedup in matrix construction in AORSA2D.
- ScaLAPAC MPP dense linear solver is very effective. Up to 68% of peak theoretical efficiency on IBM SP. Scales essentially linearly to2024 processors
- New AORSA formulation transforms from Fourier space back to configuration space – results in large reduction in matrix size and solution time
  - AORSA2D – linear solve speedup x3.7, matrix memory 1/2.5
  - AORSA3D – linear solve speedup x100, matrix memory 1/40
  - Can eliminate boundary points in conducting wall – huge savings in 3D
  - Ultimately should be able to exploit sparseness in configuration space for additional savings

3D example: Compact Stellarator

	Fourier space	Configuration space
Number of equations	248,832	39,492
Matrix size	990 Gbytes	25 GBytes
Time to load matrix	1.2 min	7.1 min
Matrix solve (ScaLAPACK	344 min	3.5 min
Fourier transform	9.5 min	0.04 min
Total CPU time	358 min	13.4 min
Flops/processor	1.1 Gflops	0.25 Gflops

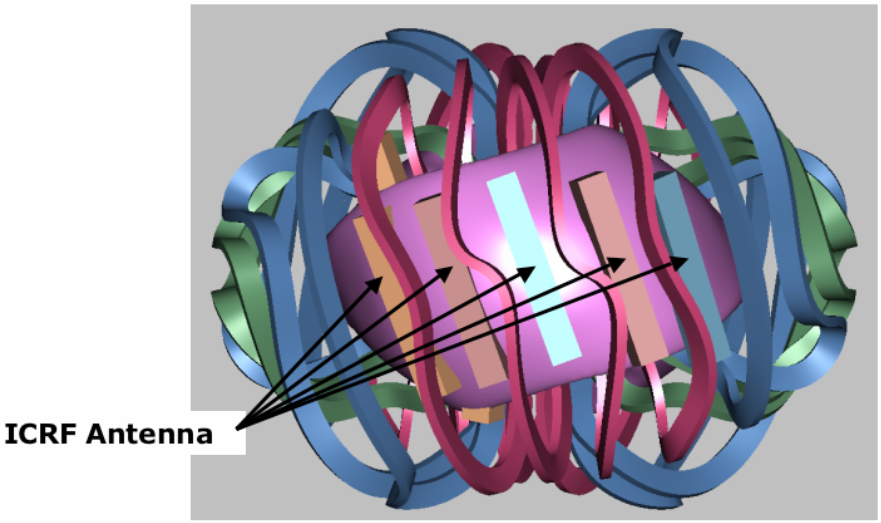
Note:

Performance improves × 27 ⇒ Total CPU time

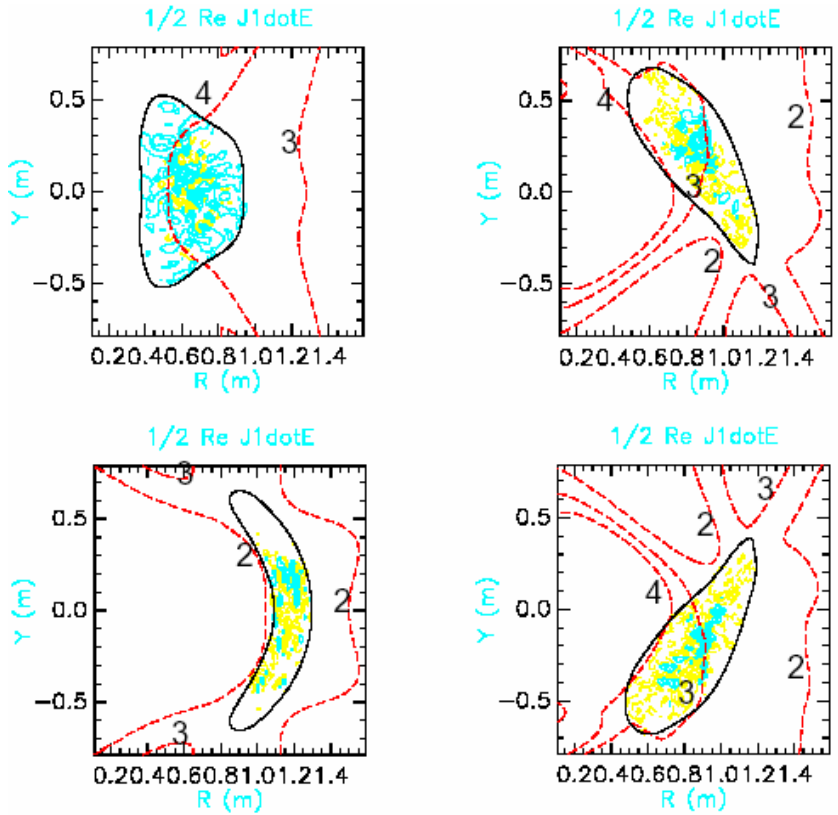
Efficiency drops/4 ⇒ Flops/processor

3D calculations with AORSA3D for high harmonic fast wave heating for QPS compact stellarator

- 2002 → One full 3D calculation of LHD
- 2003 → Now routine analysis of QPS developing viable heating scenarios, guiding machine design
- f = 42 MHz, 2 strap antenna, $T_e = T_i = 500$ ev, ne = $1.8 \times 10^{19} m^{-3}$, 64×64×64 modes



H majority heating in QPS

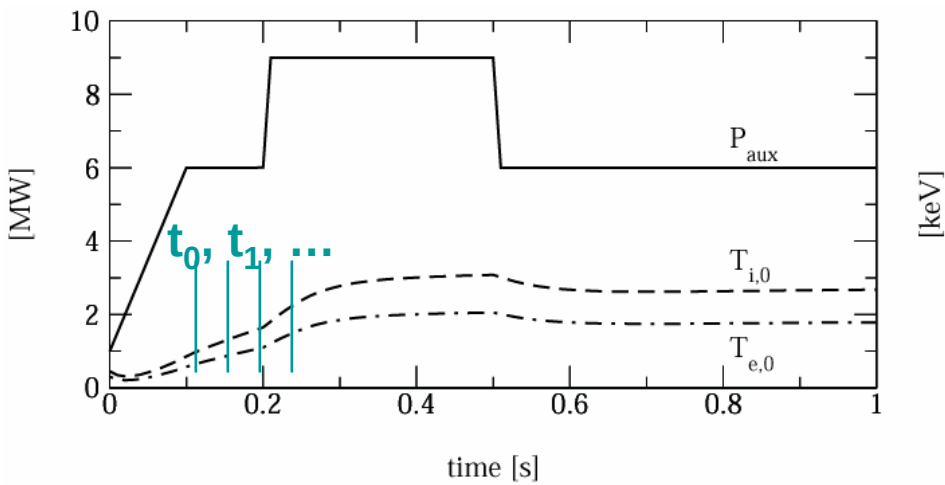


We are developing methods to accelerate RF solution for time evolving plasmas – evolutionary preconditioning

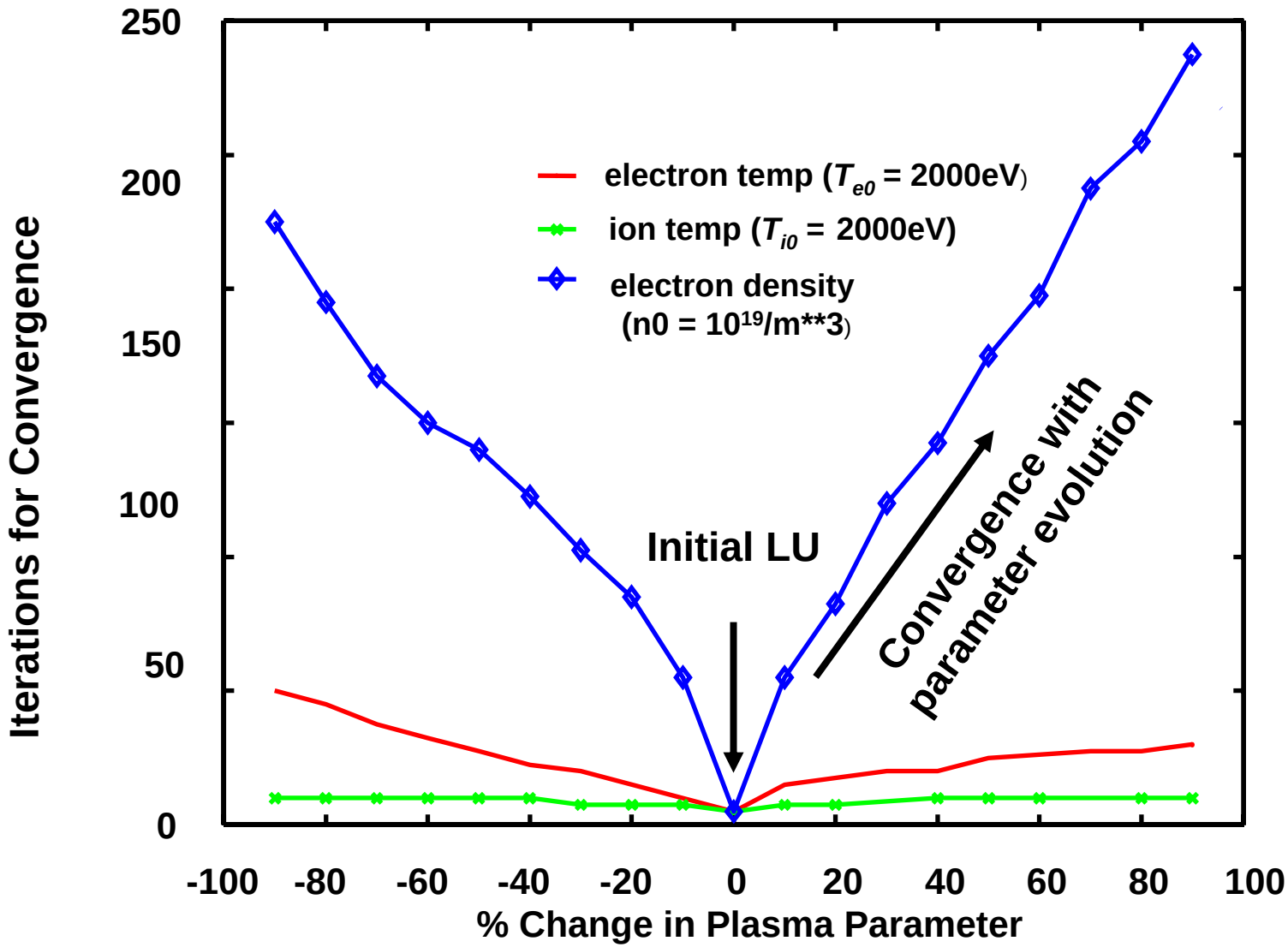
- **Direct solution of RF system matrix very expensive – $O(n^3)$**
- **RF system matrix – non-symmetric, non-positive definite ⇒ iterative solution methods not effective – $O(n^2)$**
- **However: Plasma parameters evolve slowly during a simulation => Use earlier direct solutions for preconditioning of Krylov space iteration**

t=0: exact LU factorization $O(N^3)$
$t=t_1$: iterative based on t_0 LU preconditioner $O(N^2)$
$t=t_2$: iterative based on t_0 LU preconditioner
$t=t_3$: iterative based on t_0 LU preconditioner
…

Generate a new LU preconditiner when convergence is poor.



An Exact LU Preconditioner Leads to Rapid GMRES Convergence as Plasma Parameters Evolve from Transport



Alternate approach to integration with transport code:

- **TRANSP (serial) plus TORIC (parallel)**
  - Need accurate source models for transport simulations in which mode conversion provides significant heating and/or current drive.
  - Run parallel TORIC jobs as part of TRANSP runs (which are serial.) TORIC takes longer (much longer for MC cases) to run than TRANSP.
  - A logical approach would be to schedule the TORIC job then run TRANSP in a preemptive mode.
  - TORIC would compute a time step (about 1 hour on 24 processors), then request that the TRANSP computation continue (1 to 2 minutes, serial.)
  - Data transfer needs are not large and may be handled through MDSplus (to be implemented in TORIC.)
  - **Utilize the Fusion Grid to carry out code communication**

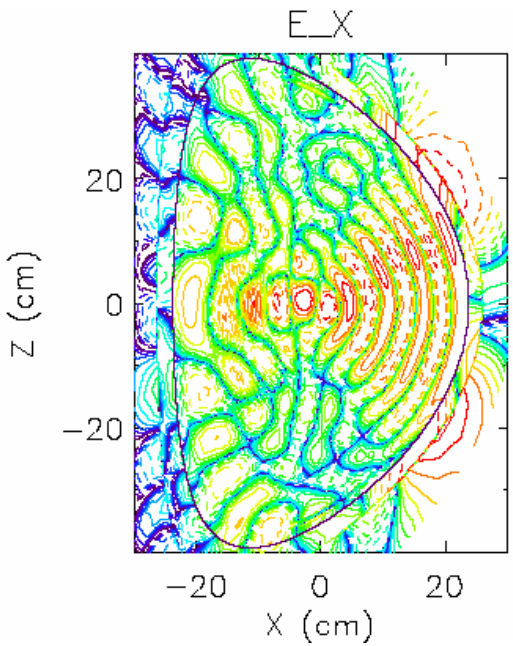
Alternate research paths are being pursued that could have high future pay-offs

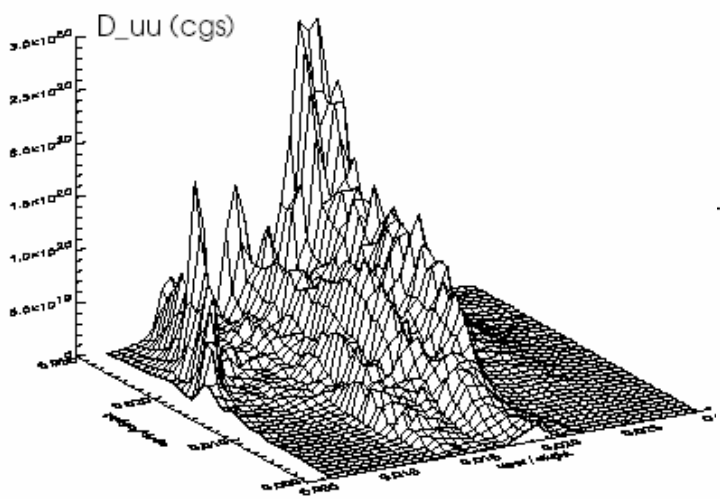
- **Calculation of quasi-linear operator by direct integration of particle orbits in 2D wave fields**

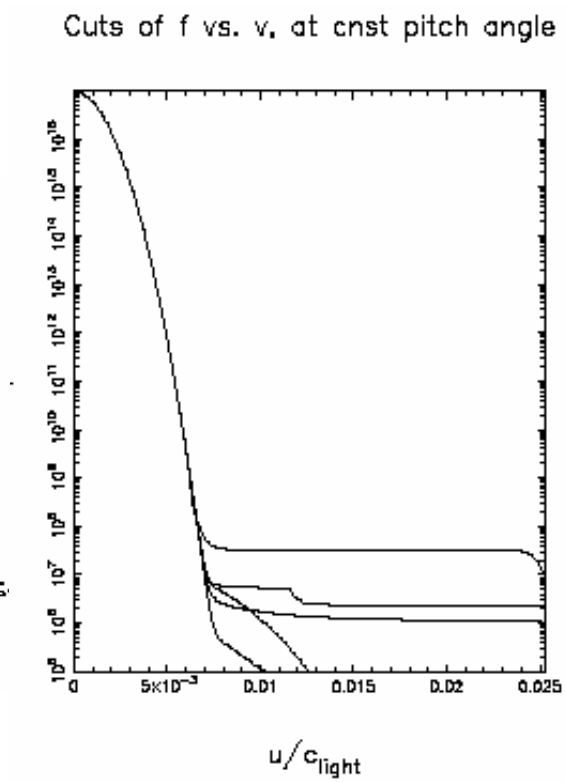
- **Exploration of alternative field basis sets – splines, wavelets, Gabor transforms**

Progress on Fokker Planck calculation of non-Maxwellian distribution and coupling to wave codes

- **Numerical integration of ion orbits with full-wave electric field solutions gives velocity space diffusion, including radial deviation from flux surface**
- **Wave fields obtained from TORIC 2D code**
- **Solution for f(r,v) obtained from CQL3D**



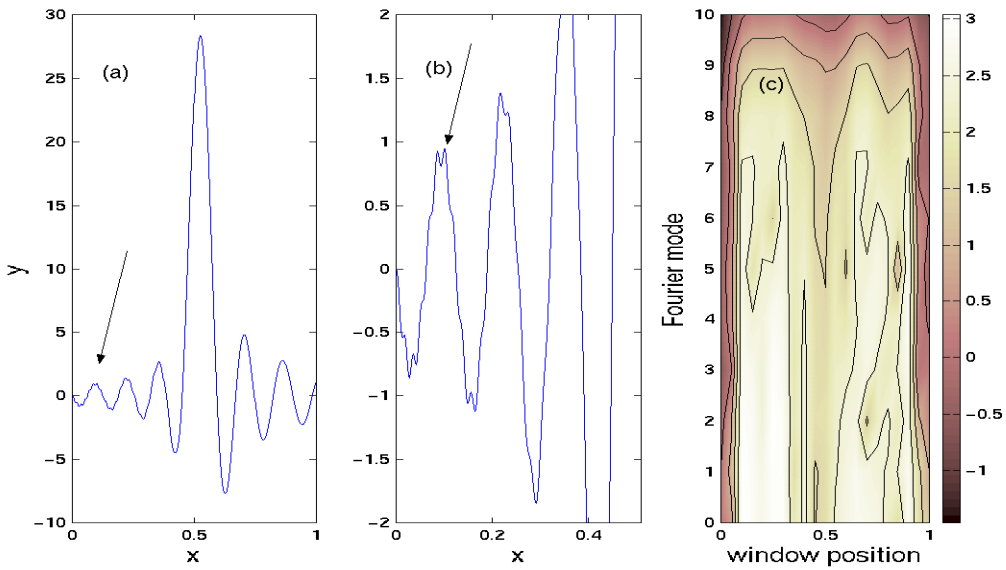


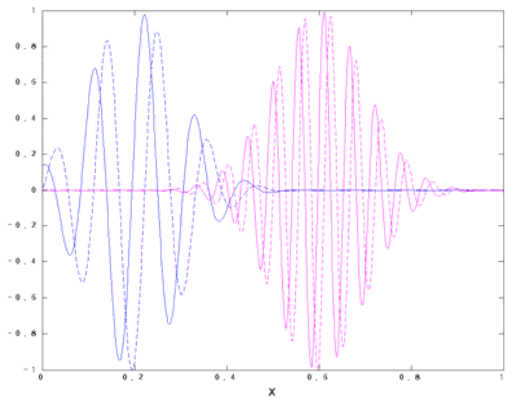


- **Computation takes ~ 3hr/flux surface on PC**
- **Benchmarking and speedup is in progress**

Progress with Gabor/wavelet field representation

- Fourier basis set implies a uniform grid
- Dielectric tensor for a Maxwellian plasma will be nearly as analytic as for Fourier basis set.
- These basis sets provide alternative approach for non-uniform adaptive grid and sparse matrices
- Combining the best of the finite element method (FEM) and FFT
  - Solution is expanded in Gabor wave packets (smooth to all orders)
  - Local boundary conditions (like FEM)
  - Can handle high order equations (e.g. mode coupling)
  - Can capture short wavelength features





Summary

- **ICRF full-wave phenomena can now be explored in 2D and 3D with much improved resolution and physics detail:**
  - **Mode conversion and fast wave heating in 2D (routine)**
  - **Fast wave heating in 3D**
  - **Effects of non-Maxwellian distribution (closed loop computation with full-wave solver is essentially done)**

- **Full-wave phenomena in the LHRF regime can now be studied for the first time ever in toroidal geometry leading to physics insights into the effects of focusing and diffraction.**

- **To make feasible the integration of advanced RF models with other disciplines, such as transport or stability, or to carry out extensive closed loop computations within RF, careful attention to code speedup and optimization will still be required:**
  - **It's amazing how much you can optimize**
  - **To accomplish what we have in this area our partnership with Computer Science and Applied math has been essential**