Scientific Progress in the SciDAC Center for Simulation of Wave – Plasma Interactions

Paul Bonoli on behalf of the SciDAC Center for Simulation of Wave-Plasma Interactions

Meeting of the PSACI Program Advisory Committee
Princeton Plasma Physics Laboratory
June 5-6, 2008

Participants in the Center for Simulation of Wave – Plasma Interactions (CSWPI)

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Report on Major Scientific Progress During the Past Year

- **Reconstruction of 3-D ICRF wave fields, from full toroidal mode spectrum of antenna loops:**
  - **Fast wave driven current density in NSTX and ITER using AORSA.**
  - **Ion cyclotron heating in Alcator C-Mod and ITER using coupled AORSA-CQL3D.**
- **Major upgrades to physics models:**
  - **Preliminary coupling of AORSA and ORBIT-RF coupling.**
  - **AORSA and time dependent CQL3D with static plasma – collaboration with SWIM FSP Project.**
  - **Successful implementation and testing of a parallel LH field solver TORLH with waveguide BC for the parallel electric field:**
    - **Simulation with resolution of 2047 (N_m) × 980 (N_r) satisfies 2008 DoE JOULE Theory Milestone.**
  - **Implementation of nonthermal ions and electrons in TORIC in preparation for closed loop coupling between TORIC and CQL3D.**
  - **Implementation of a far field sheath BC in the TORIC solver.**
- **Algorithmic and performance enhancements:**
  - **AORSA utilization of 154 TF @ 30, 000 processors on CRAY XT-4 Jaguar NLCF.**
  - **Algorithm for iterative solution of LH full-wave problem.**

Mathematical formulation of Wave Propagation and Absorption

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)

SIGMAD

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

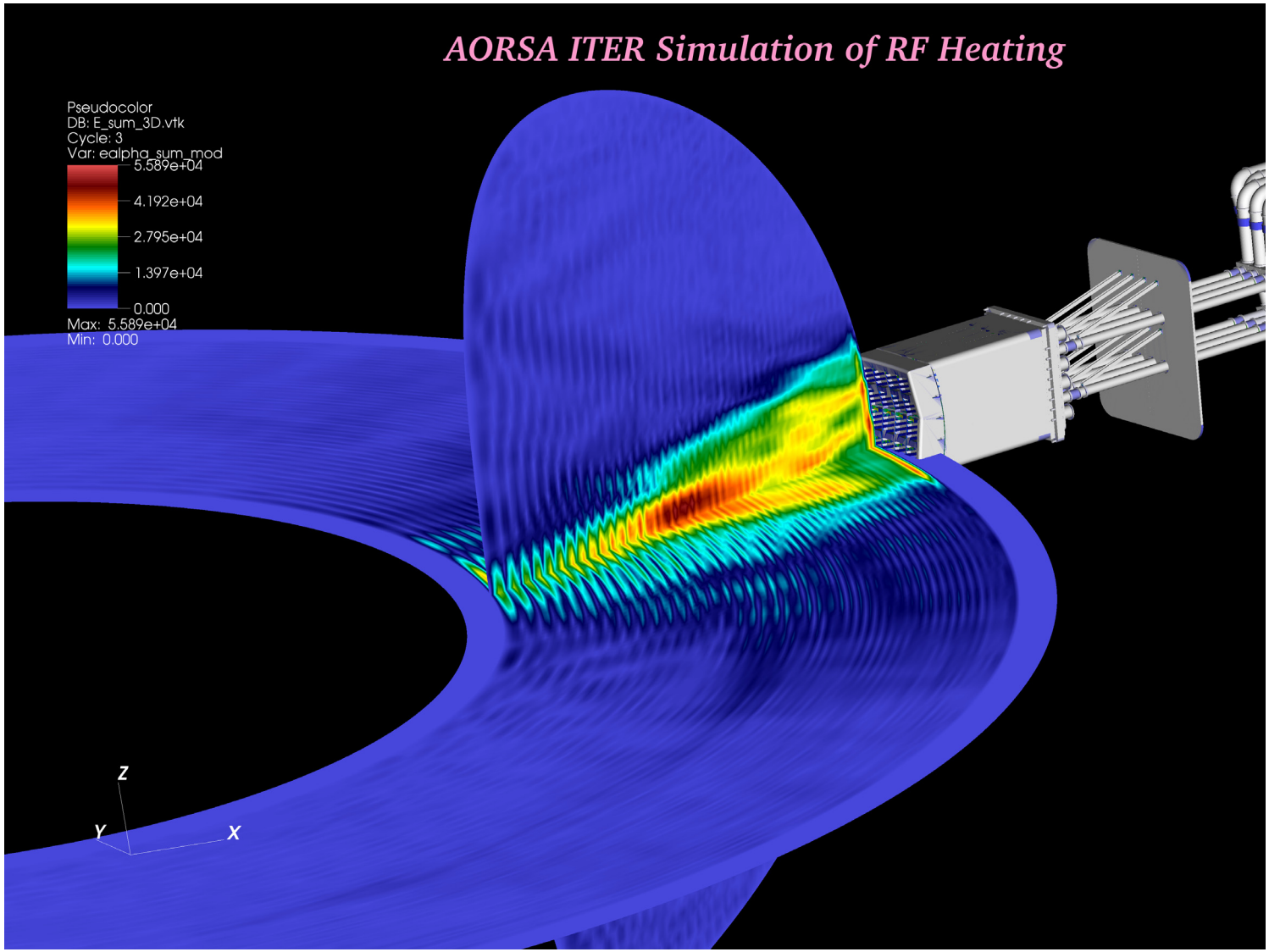
$$\frac{\partial}{\partial t}(\lambda f_0)=\nabla_{\mathbf{u_0}}\cdot\Gamma_{\mathbf{u_0}}+\langle\langle S\rangle\rangle+\cancelto{0}{\langle\langle R\rangle\rangle}\quad\text{where}\quad\nabla_{\mathbf{u}}\cdot\Gamma_{\mathbf{u}}=C(f_0)+Q(\mathbf{E},f_0)$$

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.

3-D ICRF Field and Absorption Studies

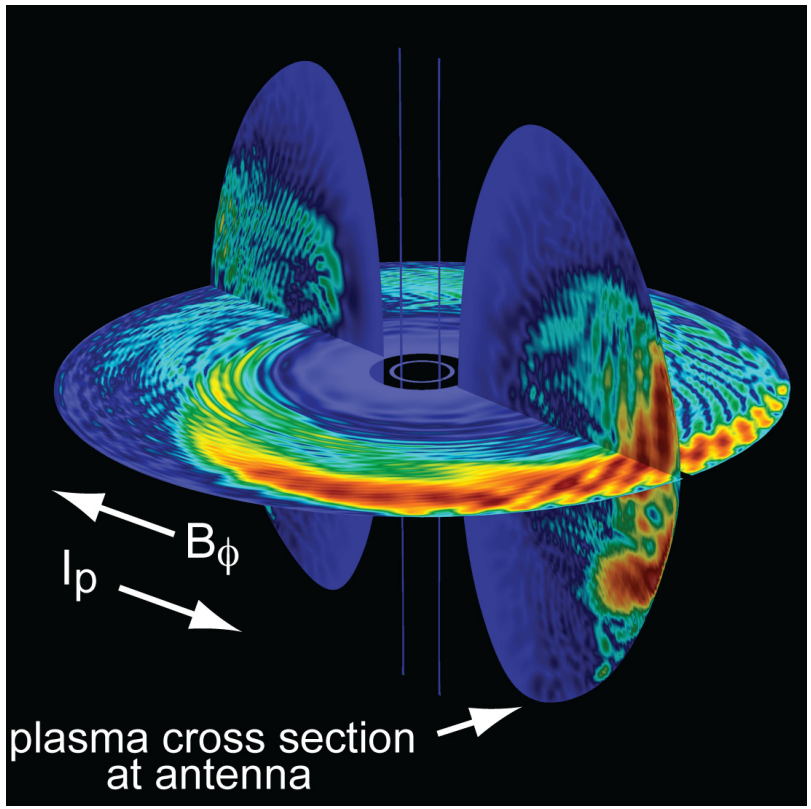
3-D visualization of the ICRF wave fields in ITER shows "hot spots" near the antenna surface where the wave amplitude is high



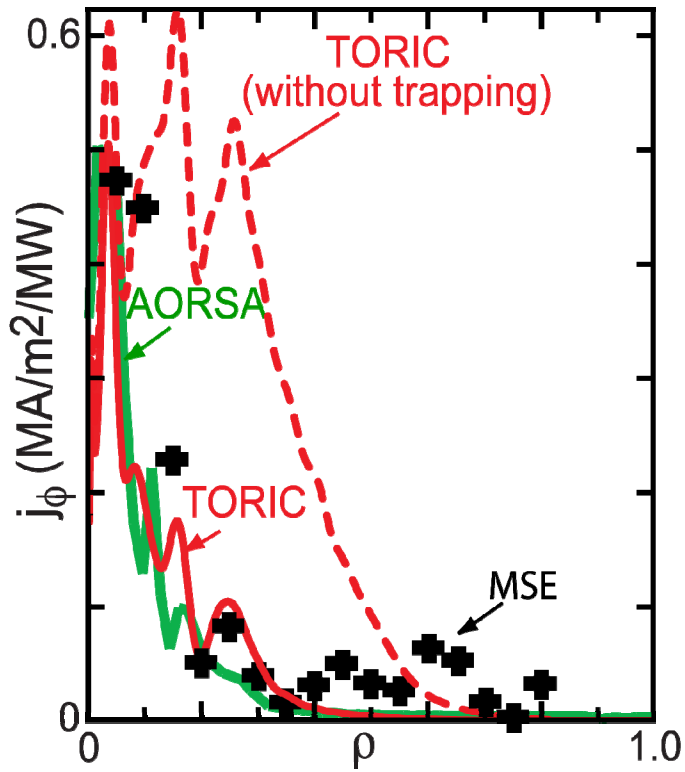
- **AORSA simulation using 100 toroidal modes of the ICRF antenna.**
- **Calculation done on 2048 processor cores in 2 hours on Jaguar facility.**

3D Reconstructions of HHFW Fields for Current Drive Calculations in NSTX

- AORSA simulation of HHFW wave fields in NSTX using 101 toroidal antenna modes ($k_{//} = 8m^{-1}$)



- **AORSA - 101 toroidal modes (26 kA)**
- **TORIC – single mode (37 kA)**
- **Experiment – (34 kA)**

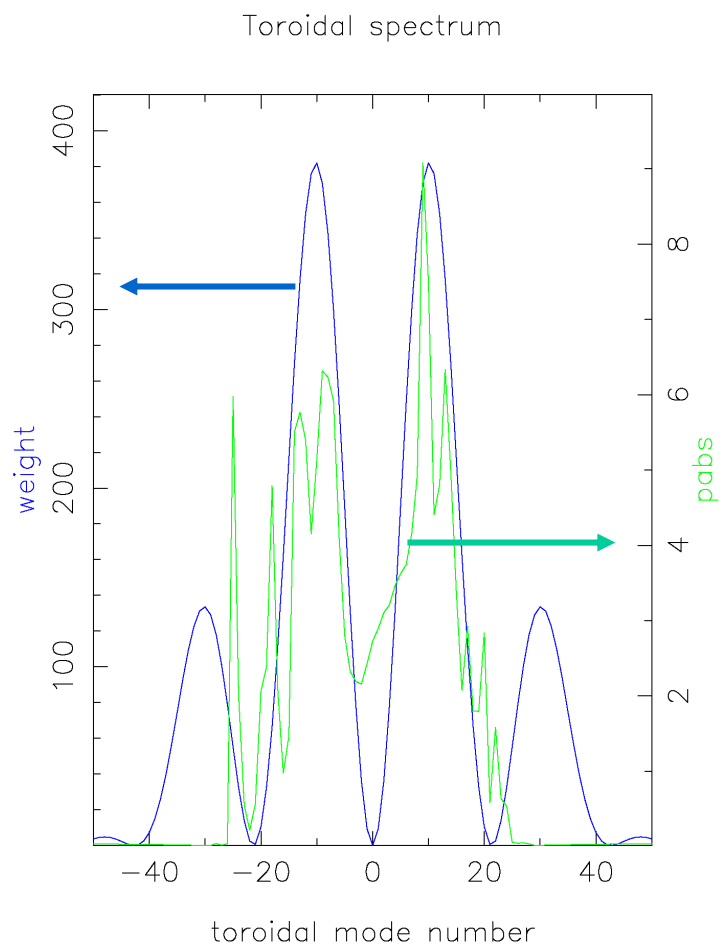


Procedure for Alcator C-Mod Minority ICRF Computation in 3-D

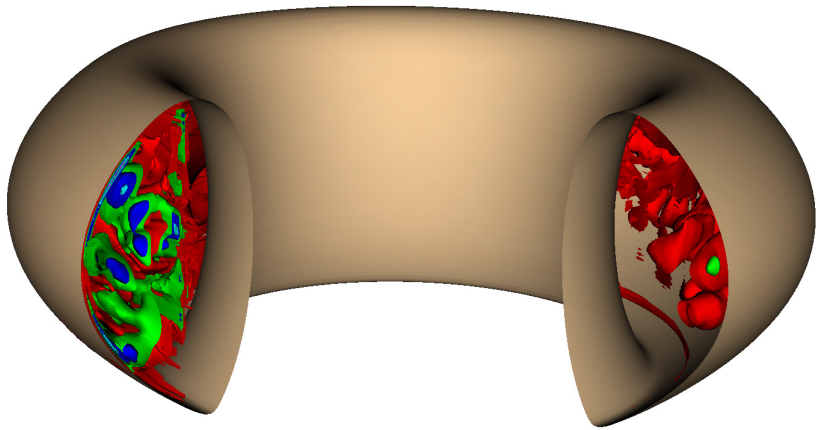
- Use 101 toroidal modes of the two strap D- and E- antennas in dipole phasing (180 degrees) to reconstruct Wdot and the quasilinear operator from the 3-D wave electric fields:
  - **Utilize 2048 processors for 8 hours on Franklin for one iteration with the Fokker Planck solver - writes a 4 GB file with D_{ql} to be summed.**
- The electric fields and W-dot are summed and scaled as usual, but this time the quasi-linear operators are also summed and scaled.
- Using the summed QL operator, CQL3D calculates the minority H distribution function consistent with the 3-D fields.
- **Process is repeated until convergence is achieved.**

At last iteration: 101 modes in C-Mod with the H distribution function for a single mode (n_φ = 10)

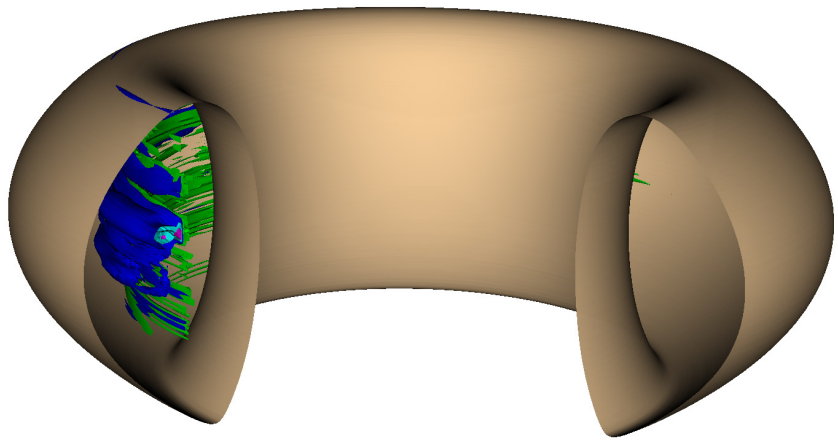
k_ϕ Spectrum



Fields

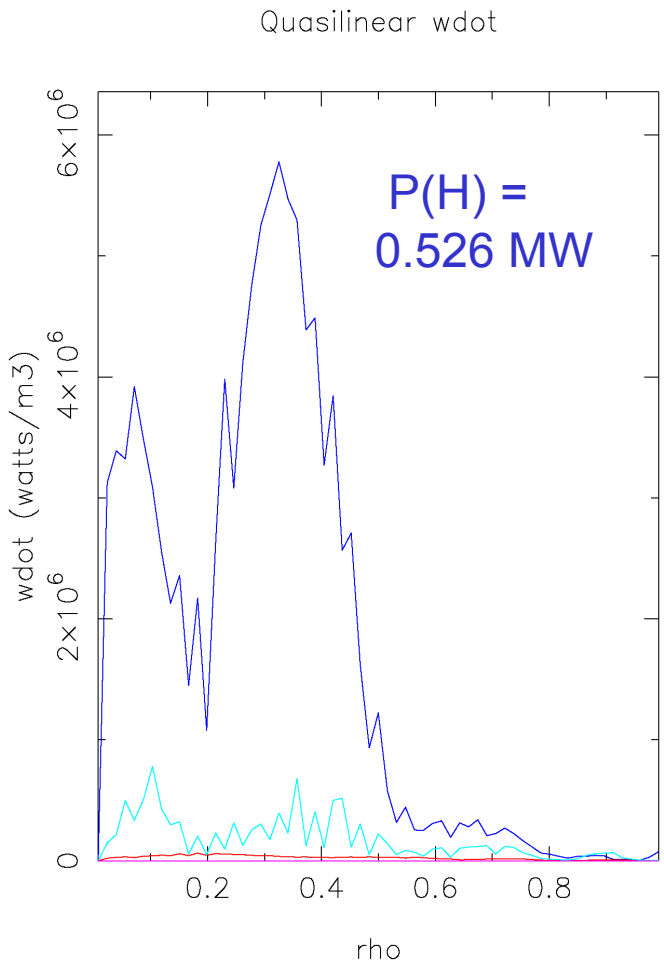


Heating

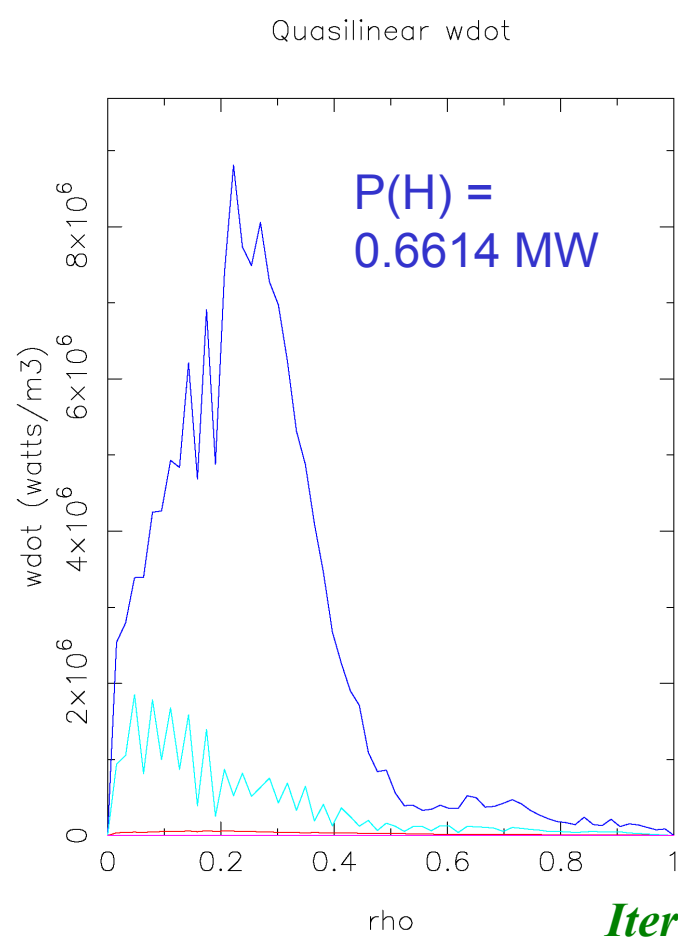


Alcator C-Mod: Full-wave (AORSA) heating profiles show differences between single and summed modes

AORSA – 2D
(n_ϕ = 10)



AORSA – 3D
(n_ϕ = -50 : 50)

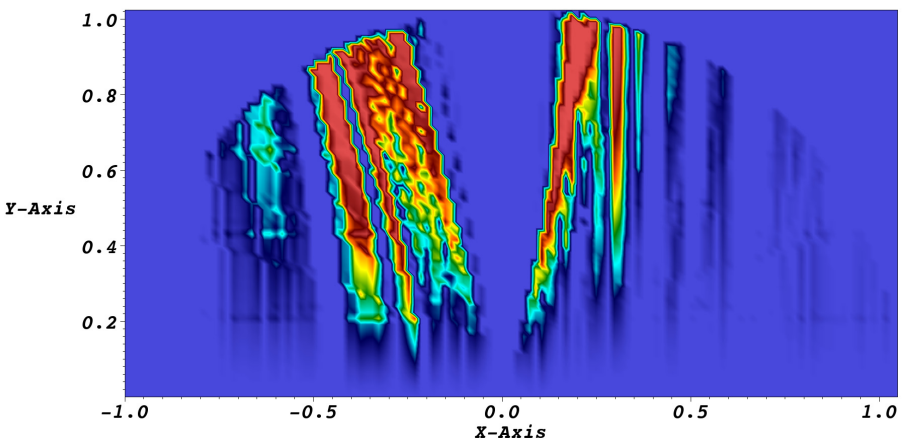


Iteration #4

Self consistent quasilinear operator (r/a = 0.306) shows significant "smoothing" of phase space structure with multiple toroidal modes -> 3D field reconstruction is to essential to see this feature!

2D: Single mode (n_φ = 10)

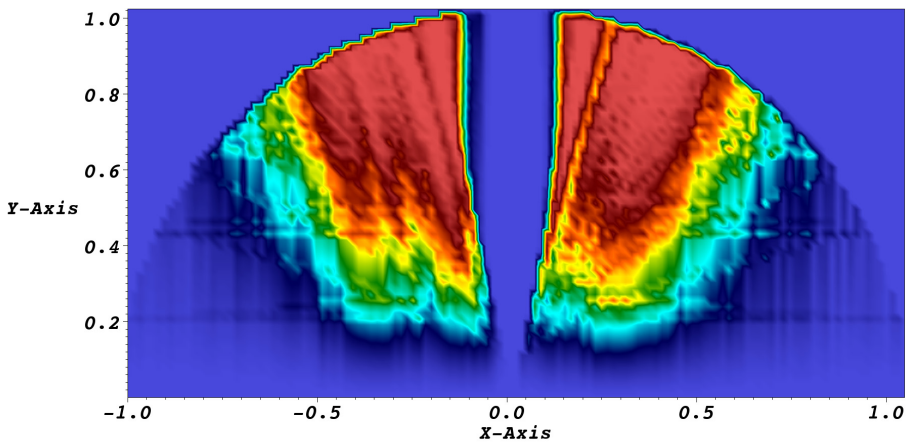
$v_\perp$ (mid-plane)



$v_{//}$ (mid-plane)

3D: All modes (n_φ = -50 : 50) weighted by 2 strap antenna

$v_\perp$ (mid-plane)



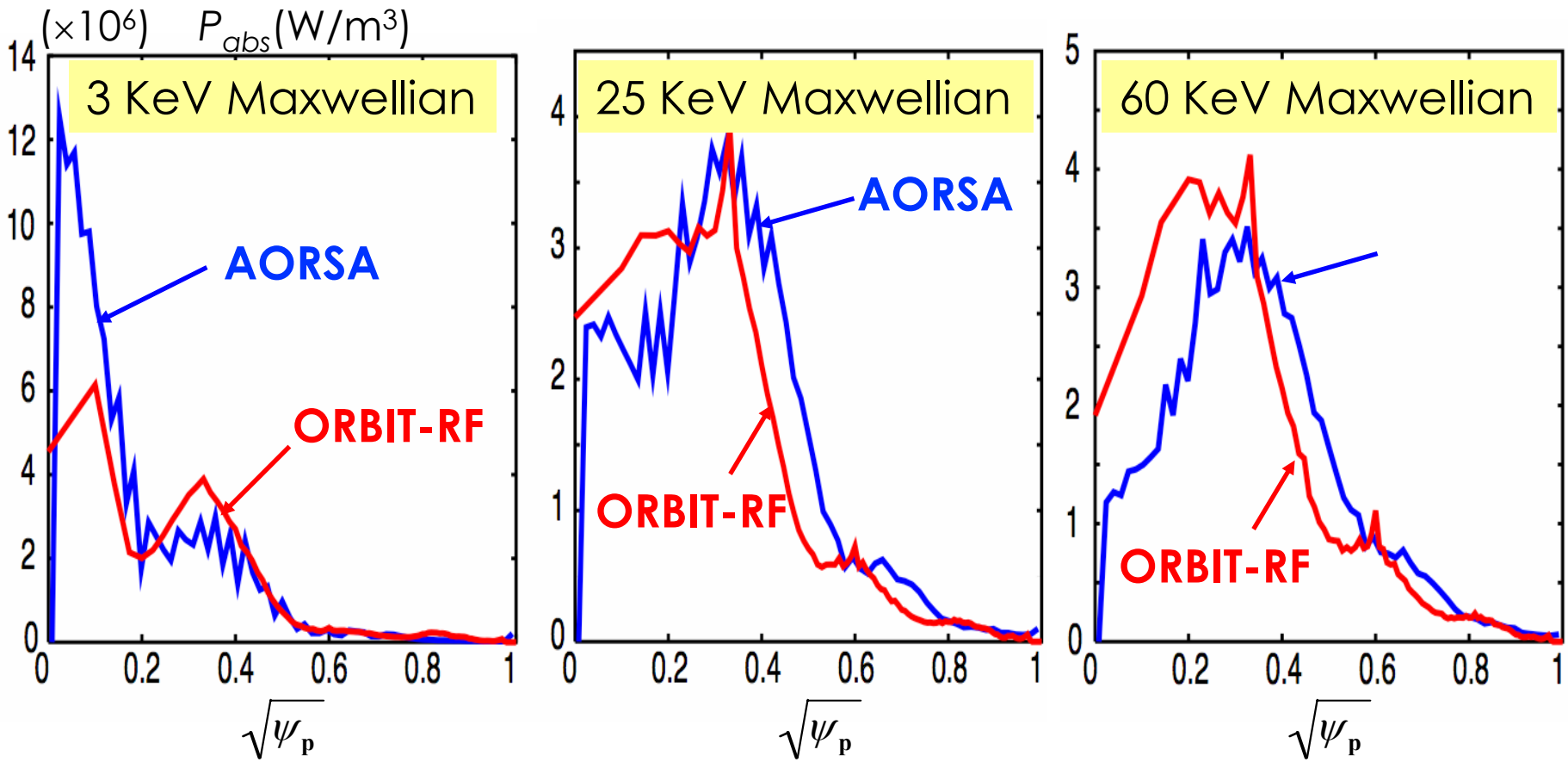
$v_{//}$ (mid-plane)

Finite ion drift orbit effects will be studied using the coupled AORSA and ORBIT-RF codes

- **The Monte Carlo code ORBIT RF has been combined with the AORSA ICRF solver for a simplified set of conditions for a minority heating case in C-Mod:**
  - **Single $k_{//} = (n_\phi / R)$ and $k_\perp$ from fast wave Disp. Rel.**
  - **AORSA computes $E_+(\sqrt{\psi_p}, \theta)$, where $\theta = \tan^{-1}(Z/(R-R_0))$, assuming a minority Maxwellian ion distribution function with temperature $T_{min.}$**
  - **ORBIT-RF determines resonance locations, evaluates $D_{ql}(E_+)$ using the AORSA fields, and then computes f_{min}**
- **Next steps:**
  - **Pass $D_{ql}(v_\perp, v_{//}, R, Z)$ to ORBIT-RF to account for $k_{//}$ exactly.**
  - **Examine best way to pass the statistical distribution from ORBIT-RF to AORSA to do self-consistent iteration.**

We find better agreement at the 0th Iterate using ORBIT-RF and AORSA after extensive verification activity*

Test particles are not updated in energy and pitch after "kicks"
Single passing of resonances for each of 1 million particles

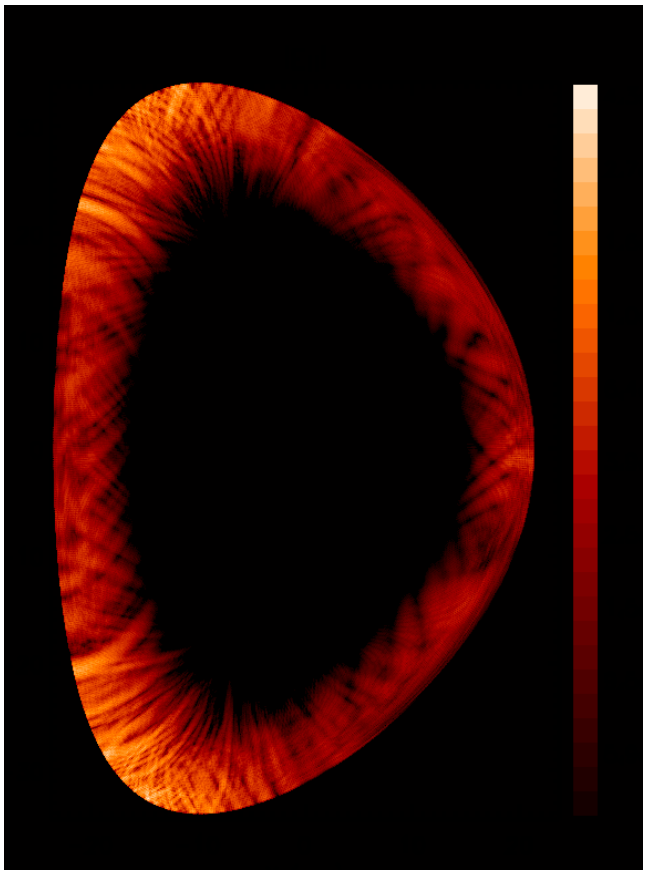


*Found differences in definitions of E_+ used in AORSA and ORBIT-RF

Full-wave LHRF Field Simulations

Full-wave LH Field Simulations have been obtained for Alcator C-Mod Parameters

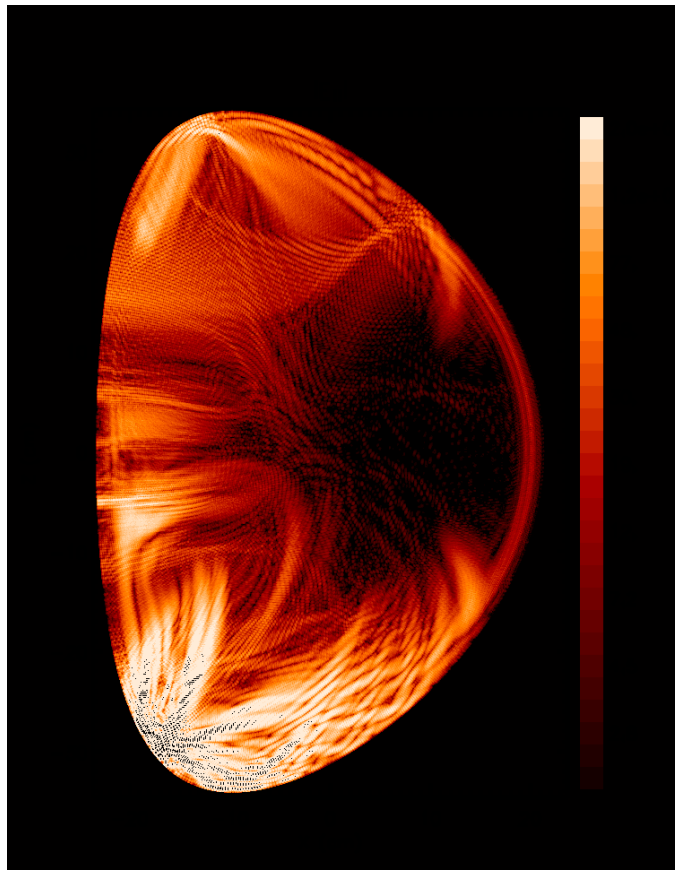
2047 (N_m) × 980 (N_r)



$n_e(0) = 7 \times 10^{19}\ m^{-3}$

$n_{//} = 1.55$ $T_e(0) = 2.33$ keV

1023 (N_m) × 980 (N_r)

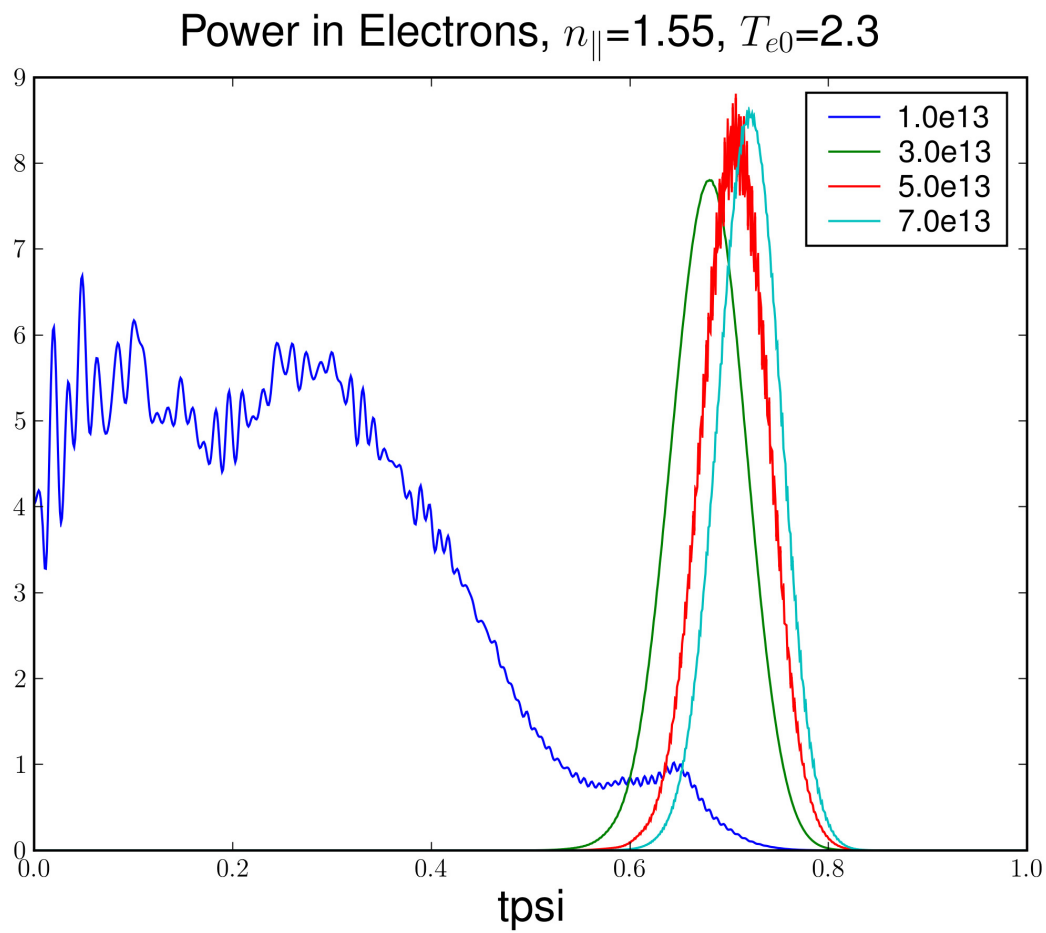


$n_e(0) = 1 \times 10^{19}\ m^{-3}$

$n_{//} = 1.55$ $T_e(0) = 2.33$ keV

Full-wave simulations show core penetration sensitive to density decrease – may be indication of sharp transition to regime where diffraction is no longer important at longer $\lambda_\perp$

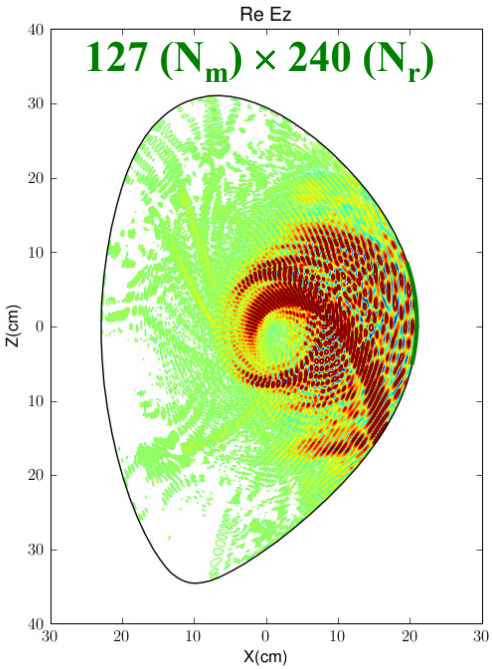
Srf
(MW/m^3/MW$_{inc}$)



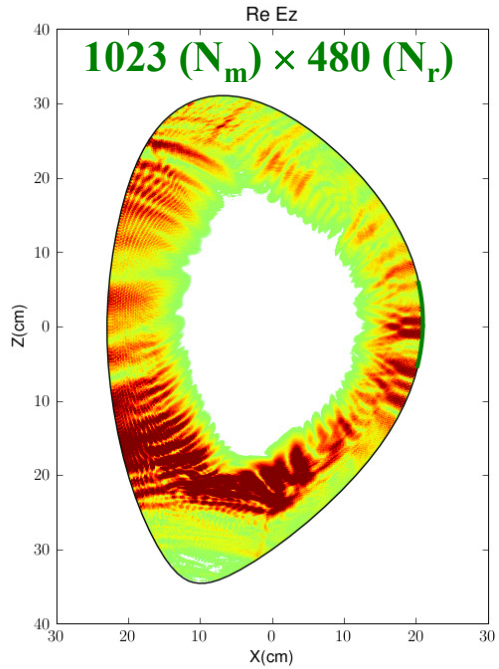
(r / a)

Intriguing Differences found between Ray Tracing and Full-Wave

Full-wave + Non-Max.



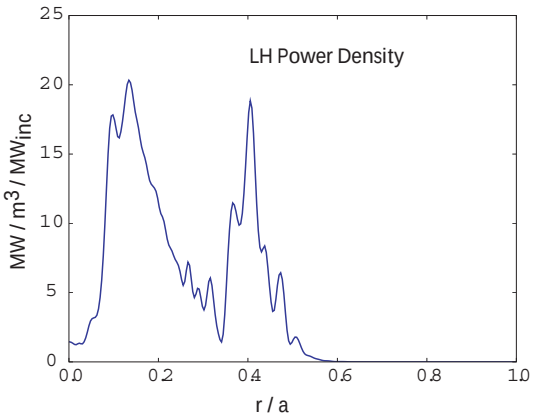
Full-wave + Non-Max.

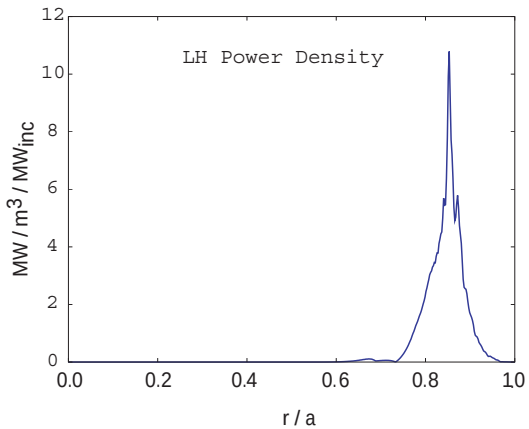


Possible reasons for differences are now being investigated:

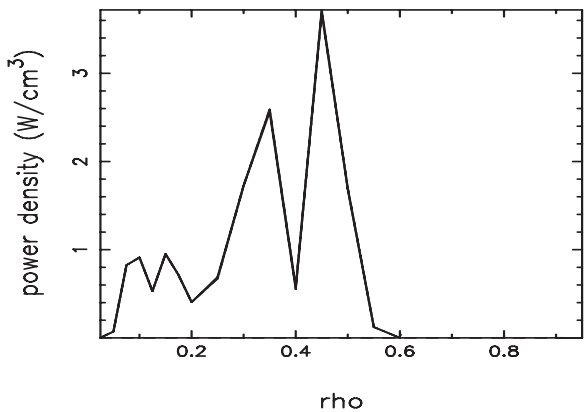
Full-wave effects such as diffraction and focussing – do beam tracing to understand.

Differences in phase front reconstruction by full-wave treatment in multi-pass regime.





Ray Tracing + Fokker Planck (GENRAY-CQL3D)



Full-wave simulations use the same EQDSK equilibrium and non-Maxwellian distribution computed by the ray tracing & Fokker Planck [$N_e(0)=0.7\times10^{19}$ m^{-3}, Te(0)=2.3 keV, B_0=5.4 T].

Nonlinear Antenna Studies

Nonlinear ICRF Antenna Sheath Work

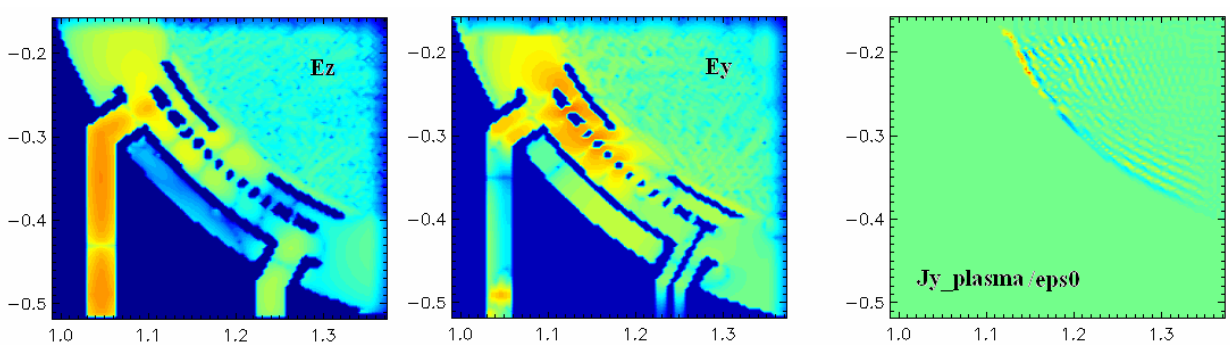
- **Goal: determine sheath potential and power dissipated in sheaths (parasitic losses) by wave energy near the wall from a sheath boundary condition (BC) in TORIC that accounts for misalignment between metal wall and B:**
  - Compute the **linear ICRF** fields from combined TOPICA-TORIC codes.
  - Proof of principle: metal wall BC with estimate of wall-magnetic field mismatch allows estimate of sheath potential and resulting power dissipation in sheaths
  - Full implementation: iterate TORIC fields until **nonlinear sheath BC** is satisfied; compute sheath power dissipation from converged fields.

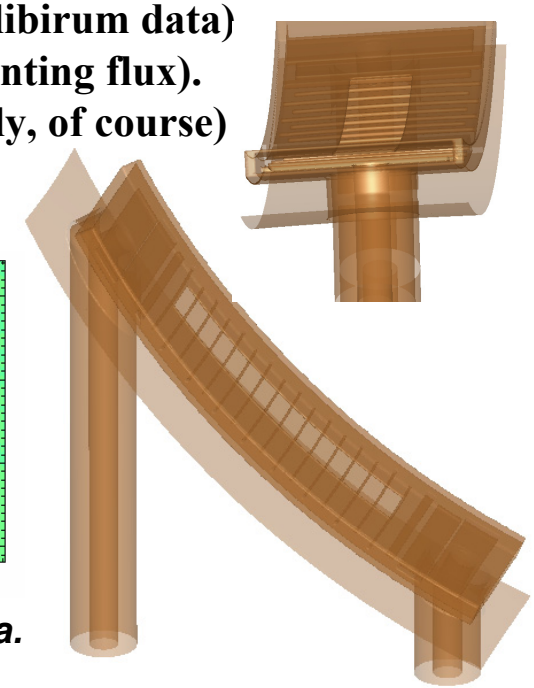
- **Investigate sheath dissipation for minority heating schemes in C-Mod:**
  - Strong single pass damping – D (H)
  - Weak single pass damping – D (3He)

Time Domain LHRF Plasma Simulations

- **Time domain simulations using 3D EM field solver – VORPAL**
  - **Fully implicit time domain dielectric response module has been implemented for electrons and ions.**
  - **Use PIC-treatment for ion response (fully nonlinear).**

- **Has found use outside SciDAC RF, in support of LHRF MST experiment**
  - **Providing opportunity for more feedback, debugging, verification, and validation.**
  - **LH launcher analysis, with fully realistic detail of all components.**
  - **Up to 24 million cells on local Madison cluster (34 CPU's, 136 Gig memory total).**
  - **Realistic plasma (based upon parametric fit to EQDisk equilibirum data)**
  - **Engineering diagnostics added & validated (Bdot-loops, Poynting flux).**
  - **Benchmarking against Microwave studio (vacuum cases, only, of course)**
  - **May serve as test-bed for Tech-X's new ADI algorithm.**

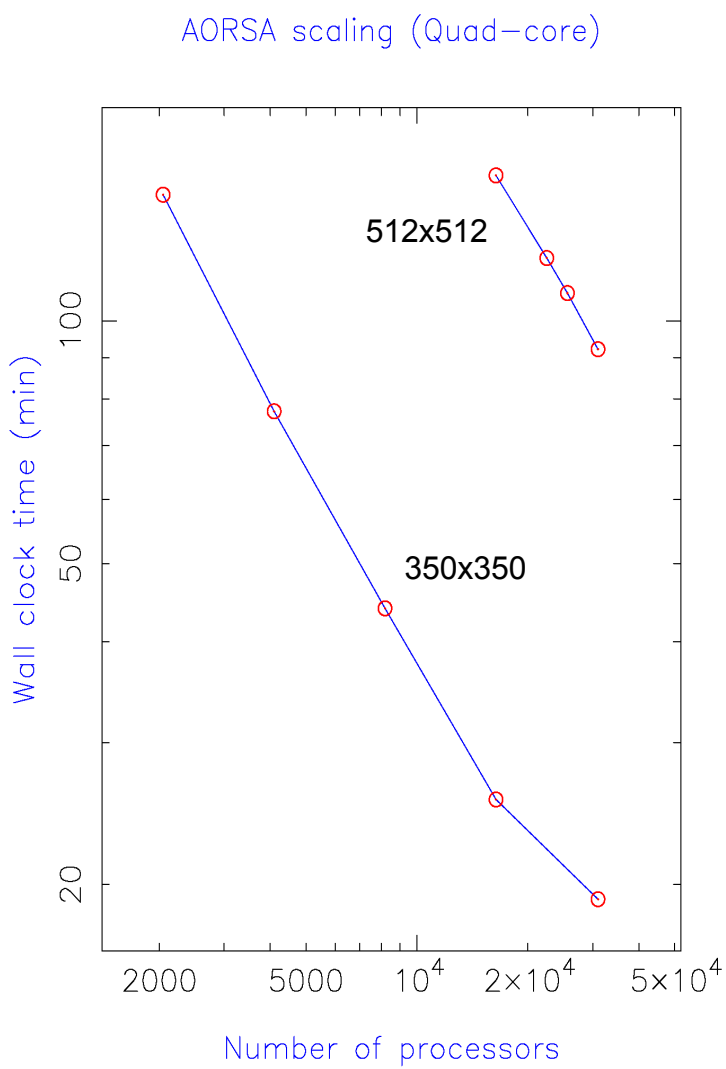


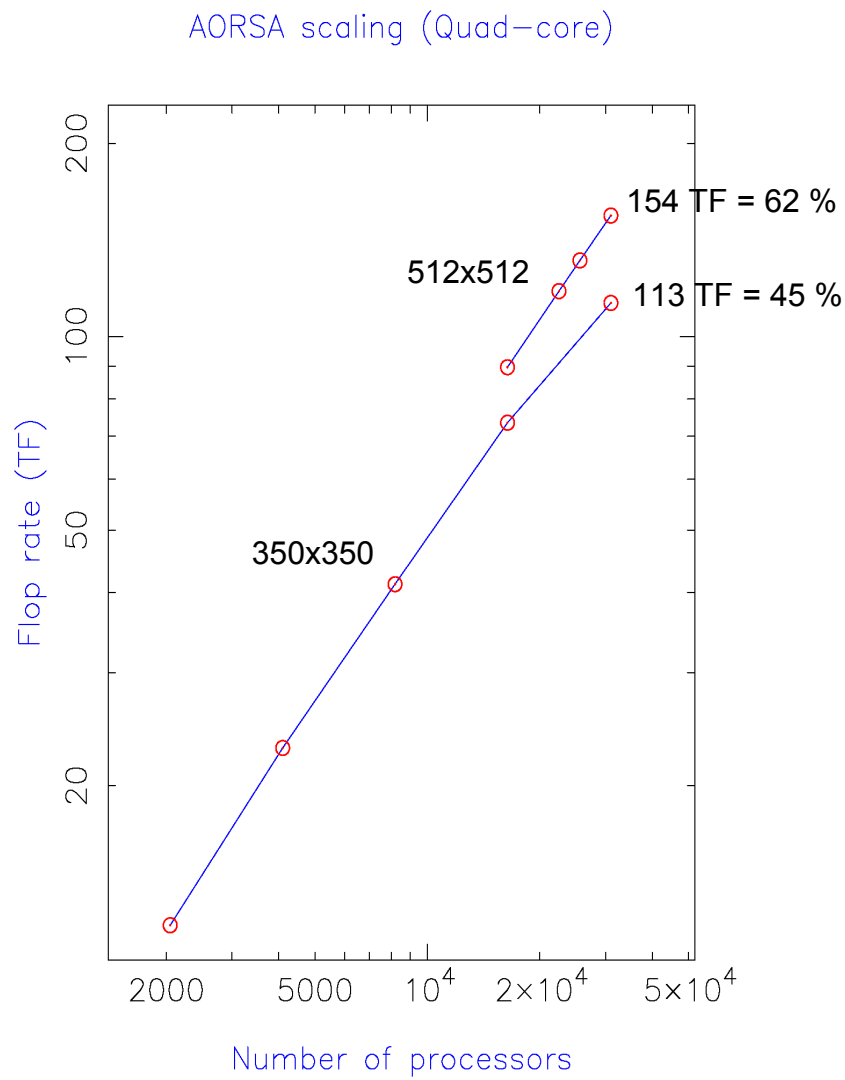


Plots show electric field and plasma current at midplane of MST antenna. 3-D simulation geometry shown at right.

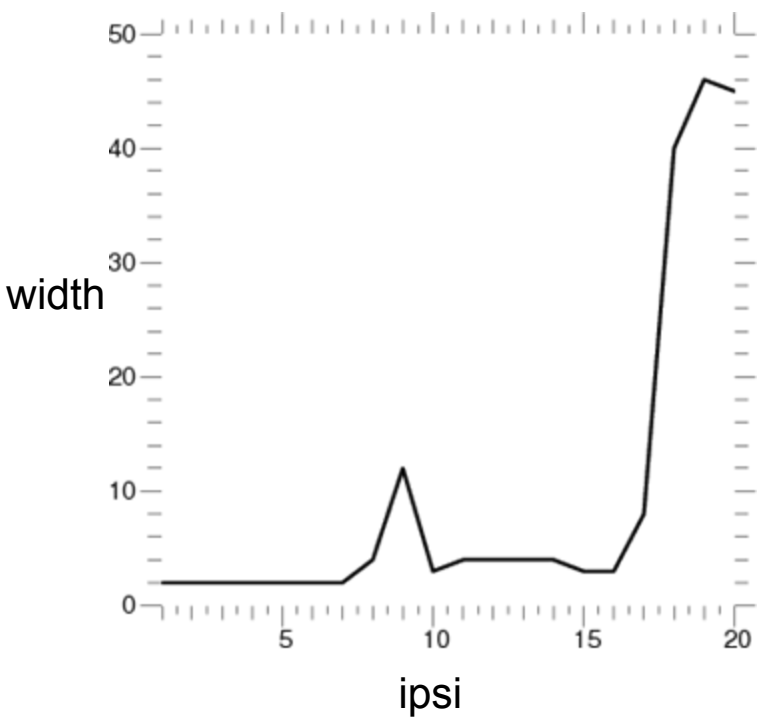
Performance Enhancements and Algorithmic Improvements

AORSA scaling on the quad-core Cray XT-4 (Jaguar)
ITER Benchmark ($2\Omega_{CT}$ and ^{3}He, $n_\varphi = 27$)
SSE optimization essential to retain linear scaling





Sparsity of the wave operator in LHRF may permit ITER scale problems



Block width is very small except at boundary. Typical block size would be in the 1000s (in this case it's 124).

- The TORLH stiffness matrix is block tridiagonal.
- The equilibrium poloidal variation is smooth, coupling m to $m' = m \pm j$, with $j << m$, *i.e.*, the block matrices are banded with bandwidth $\Delta m << m$.
- A test solver has been implemented to take advantage by decomposing blocks to banded blocks and solving iteratively.
- Operation count is reduced from $O(m^3)$ to $O(\Delta m)^2 m$. Convergence takes a few iterations.
- To do: test scaling to larger relevant sized problems, introduce sparse representation.

Summary

- Capability has been developed for relatively routine reconstruction of 3-D ICRF wave fields, from full toroidal mode spectrum of antenna loops:
  - Fast wave driven current density in NSTX and ITER using AORSA.
  - Ion cyclotron heating in Alcator C-Mod and ITER using coupled AORSA-CQL3D.
- Major upgrades to physics models were completed:
  - Preliminary coupling of AORSA and ORBIT-RF coupling, including extensive verification tests through an inter-code comparison.
  - AORSA and time dependent CQL3D simulations were performed for C-Mod minority heating: – (collaboration with SWIM FSP Project):
    - Simulations will be repeated for DIII-D and NSTX HHFW – fast ion interaction experiments.
  - Successful implementation and testing of a parallel LH field solver TORLH with waveguide BC for the parallel electric field:
    - Simulation with resolution of 2047 (N_m) × 980 (N_r) satisfies 2008 DoE JOULE Theory Milestone.
  - Implementation of nonthermal ions and electrons in TORIC in preparation for closed loop coupling between TORIC and CQL3D.
  - Implementation of a far field sheath BC in the TORIC solver.

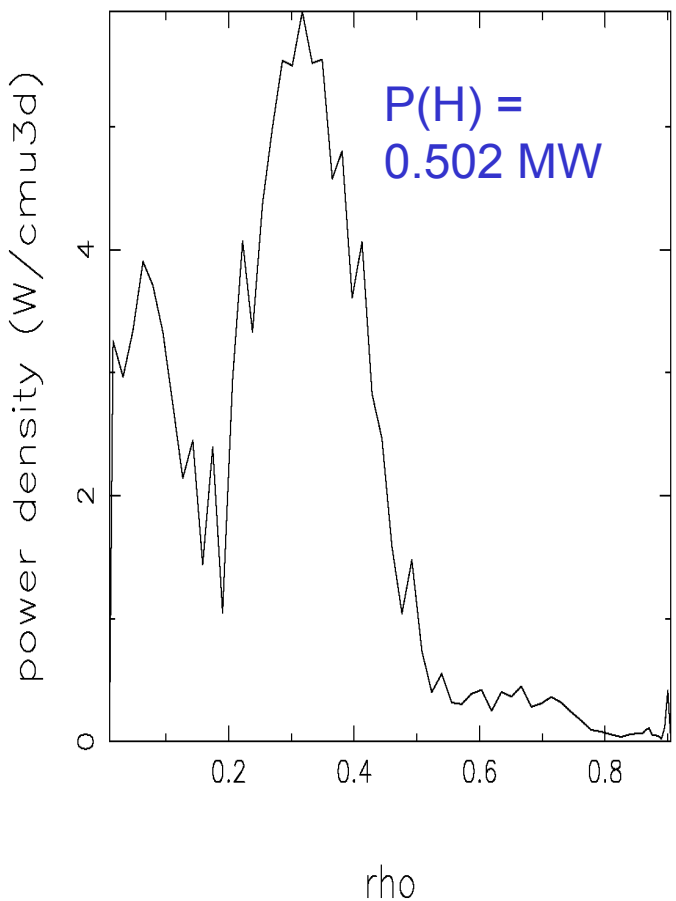
Summary

- **Achieved performance enhancements and initiated algorithmic improvements:**
  - **AORSA utilization of 154 TF @ 30, 000 processors on CRAY XT-4 Jaguar NLCF.**
  - **Studies of iterative solution techniques for the LH full-wave problem were started.**
- **New collaborations with SAP Projects will start very soon:**
  - **E. D'Azevedo (ORNL):**
    - **Work on ORBIT-RF coupling to full-wave codes**
      - **Transfer of "noisy" statistical distribution functions to full-wave solvers.**
      - **Transfer of large data sets (D_{ql} in 4D) from full-wave to orbit code.**
    - **Iterative solver techniques for full-wave LH field solver.**
  - **A. Sanderson (University of Utah):**
    - **Reconstruction of 3-D electric fields from ICRF antennas.**
    - **3-D mapping of field lines from ICRF antennas to vessel structure (for RF sheath studies).**

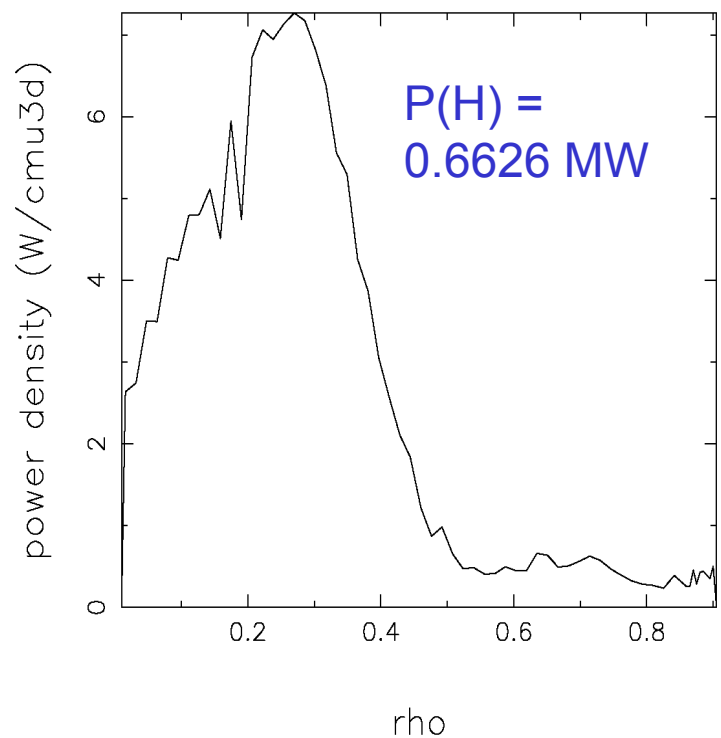
Back Up Material and Fire Drills

Alcator C-Mod: Fokker Planck (CQL3D) heating profiles show differences between single and summed modes

CQL3D – 2D
(n_ϕ = 10)



CQL3D – 3D
(n_ϕ = -50 : 50)



Iteration #4

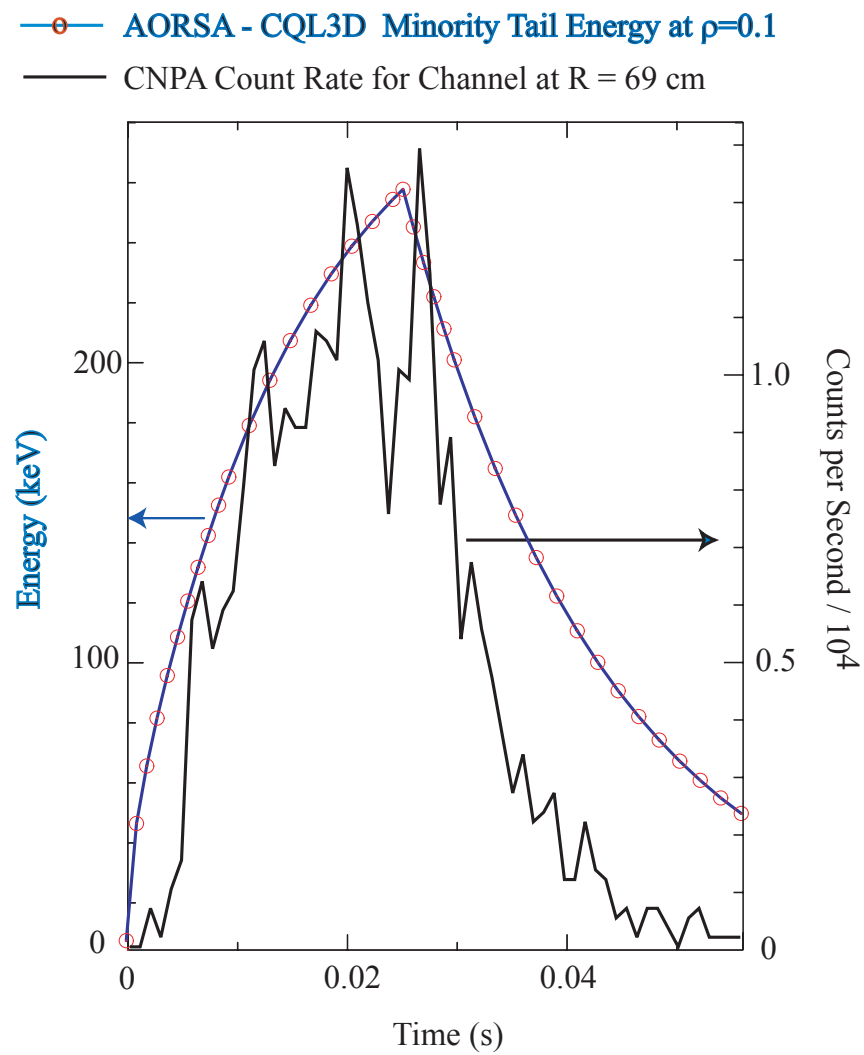
Time Dependent AORSA – CQL3D Simulation Performed for Minority Tail Formation in Alcator C-Mod Case Using the SWIM Framework

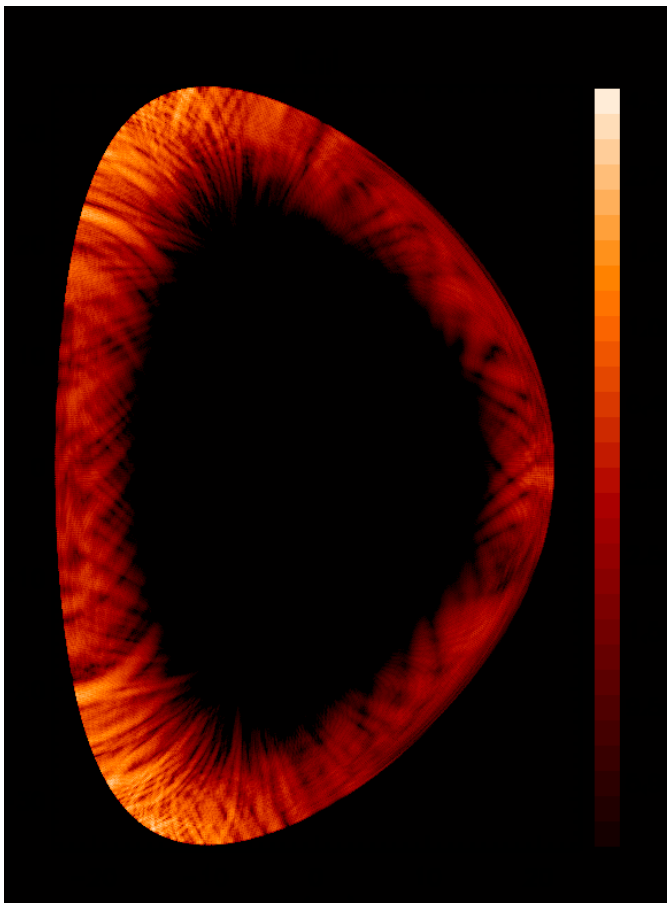
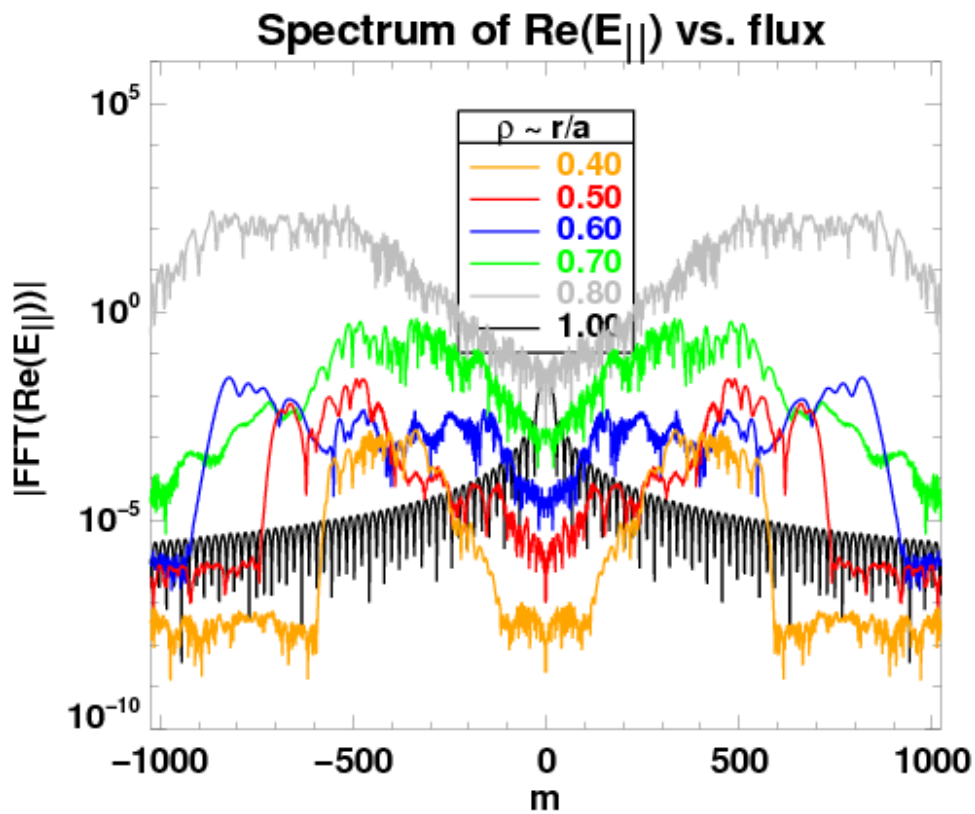
P_{icrf} = 2.65 MW @ 80 MHz

Square wave pulse for ICRF power [30 ms-on and 30 ms-off.

CNPA count rate binned over successive square wave pulses to increase signal-to-noise.

Good agreement on tail turn-on. Agreement not good on tail decay time (no spatial losses included in CQL3D simulation).



Convergence of LH wave fields demonstrated - Satisfies 2008 JOULE Theory Milestone -

- **Must retain enough poloidal modes to resolve the electron Landau resonance limit of $\omega / (k_{//} v_{te}) \approx 2.5$:**
- **$n_{//} = 1.55$, $N_m = 2047$, $N_r = 980$, 10^4 cpu-hours @ 256 processor cores**