Evolution of nonthermal particle distributions in radio frequency heating of fusion plasmas

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Abstract. Progress is reviewed on the simulation of wave-particle interactions in the ion cyclotron range of frequencies (ICRF). Two important aspects of this problem are described. First, mode conversion from a long wavelength fast magnetosonic wave to short wavelength ion Bernstein waves (IBW) and ion cyclotron waves (ICW) is simulated and validation tests of the simulations against experiment are presented. Second, simulations of the quasilinear evolution of nonthermal ion tails during the minority heating are reviewed and experimental validation tests are also discussed. In this paper we describe how access to teraflop computing capability has made it possible to advance the state of the art in this area. We also discuss two aspects of the wave-particle interaction where future work is needed and where in particular access to sub-petaflop and petaflop computing capability would be highly desirable. This work involves the interaction of ICRF waves with energetic neutral beam ions at high ion cyclotron harmonic number and addresses the inclusion of finite ion drift orbit effects in the nonthermal ion tail evolution and the inclusion of nonlinear effects such as RF sheaths in the antenna–edge plasma coupling.

1. Introduction

Early applications of RF power in plasmas employed injected waves in the ion cyclotron range of frequencies (ICRF), electron cyclotron range of frequencies (ECRF), and lower hybrid range of frequencies (LHFR) for bulk plasma heating [1]. Later, both lower hybrid (LH) and electron (EC) waves were used successfully for noninductive maintenance of the entire plasma current [2, 3]. More
recent applications have utilized LH current drive (LHCD) waves for localized control of the plasma current and pressure profiles [4, 5] and EC current drive (ECCD) for control of neoclassical tearing modes (NTM’s) [6]. ICRF-generated energetic particles have been used for control of sawteeth [7] and mode converted ICRF waves have also been considered for the generation of sheared flows for control of the pressure profile [8] and for localized control of the current profile in order to control sawteeth [9]. Current and pressure profile control is considered crucial for access to high confinement (i.e., advanced tokamak) regimes with high bootstrap current fractions (> 70%) [10]. Many of these RF heating and control applications are planned for the upcoming ITER device and in order to insure success of these RF applications in ITER, a predictive capability is needed. In particular, the recent availability of massively parallel computing platforms has made it possible to perform simulations of complex wave-particle interactions in the ion cyclotron and lower hybrid range of frequencies.

One of the outstanding challenges in performing these simulations arises from the multiple spatial scales that exist when fast ICRF waves mode convert to electrostatic ion Bernstein waves (IBW) or electromagnetic ion cyclotron waves (ICW) or when RF sheaths form in the tenuous edge plasma. Furthermore, RF waves interact in a nonlinear fashion with thermal and nonthermal particles in the plasma. This can happen when nonthermal electron and ion distributions are produced by the RF wave itself or when nonthermal ions are already present in the plasma due to neutral beam injection (NBI) and fusion reactions (alpha particles). Finally, a complete description of the wave-particle interaction involves integrating “separate” calculations for antenna coupling (linear and nonlinear response), wave propagation, and wave absorption. In this paper we describe significant progress that has been made in addressing these challenges through the use of massively parallel computing architectures, with a focus on the problem of minority ICRF heating in a tokamak.

2. Physics of ICRF Mode Conversion and Minority Heating

The physics of ICRF minority heating and mode conversion in a tokamak plasma can be summarized using the dispersion relation shown in Fig. 1, where the square of the perpendicular (to the applied magnetic field B) wave number has been plotted versus the major radial coordinate. The situation depicted in Fig. 1 was first described by Stix [11] and is known as the ion-ion hybrid resonance. A fast magnetosonic wave is coupled through an antenna at the low field side (LFS) of the tokamak denoted by R_o + a, where R_o (a) are respectively the major radius (minor radius) of the tokamak. The plasma ion species mix is primarily deuterium (D) with a dilute “minority” component of hydrogen (H). The frequency of the incoming fast wave (f_0) is chosen to match the cyclotron frequency of the minority (H) species so that the wave electric field has a left circularly polarized component that matches the polarization of the minority ion [12], resulting in absorption of the wave energy at the (H) cyclotron resonance layer (see Fig. 1). Closer inspection of the region around the cyclotron layer reveals that just beyond this layer the fast wave encounters a cut-off (k_⊥ = 0). The fast wave can then tunnel through this cut-off and is transmitted as a fast wave on the tokamak high field side (HFS) and simultaneously undergoes mode conversion to a short wavelength electrostatic ion Bernstein wave (IBW). The distance between the cut-off and cyclotron resonance is directly proportional to the minority species concentration. The presence of this mode conversion layer modifies the electric field polarization of the fast wave near the cyclotron resonance, thus playing an important role in the minority cyclotron absorption physics. Until the advent of massively parallel computing architectures it was not possible to resolve the polarization of the minority ion [12], resulting in absorption of the wave energy at the (H) cyclotron resonance layer (see Fig. 1). Closer inspection of the region around the cyclotron layer reveals that just beyond this layer the fast wave encounters a cut-off (k_⊥ = 0). The fast wave can then tunnel through this cut-off and is transmitted as a fast wave on the tokamak high field side (HFS) and simultaneously undergoes mode conversion to a short wavelength electrostatic ion Bernstein wave (IBW). The distance between the cut-off and cyclotron resonance is directly proportional to the minority species concentration. The presence of this mode conversion layer modifies the electric field polarization of the fast wave near the cyclotron resonance, thus playing an important role in the minority cyclotron absorption physics. Until the advent of massively parallel computing architectures it was not possible to resolve the electric fields of the fast wave and IBW simultaneously in the mode conversion region, including the 2D (r, \theta) tokamak geometry [8, 13].

Typically n_MIN / n_e may be less than 5% during minority heating so that a highly nonthermal particle distribution or “tail” develops as the fast wave damps all of its power into relatively few plasma ions. The presence of this tail further complicates the minority heating physics since the
plasma response must be recalculated using the new nonthermal particle distribution [14]. The modified plasma response must then be used to re-solve the electromagnetic field equations (full-wave solution) for the ICRF electric fields. The new fields are then used in a quasilinear evolution equation for the particle distribution. Again, with recent advances in large scale computing it is now possible to carry out the highly nonlinear iteration between the wave solvers and particle evolution equation in order to achieve convergence [15, 16].

\[ k_{\perp}^2 - \lambda_{\perp}^{-2} \]

\[ \text{Major Radius} \quad R_0 \quad R_0 + a \]

Figure 1: Dispersion relation for ICRF minority heating in a tokamak plasma.

3. Simulation of ICRF Mode Conversion and Model Validation

3.1. Full-wave solvers

Wave fields in the minority absorption scenario are simulated using two full-wave electromagnetic solvers. Both codes consider a rapidly oscillating wave field \( E \) with frequency \( \omega \), in which case Maxwell’s equations reduce to the Helmholtz wave equation:

\[
-\nabla \times \nabla \times E + \frac{\omega^2}{c^2} E + \frac{i}{\omega} \sigma \mathbf{J}_p = -i\omega \mu_0 \mathbf{J}_{\text{ant}}
\]  

(1)

where the plasma current \( \mathbf{J}_p \) is, in general, a non-local, nonlinear, integral operator on the electric field with a conductivity kernel that is given by:

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

(2)

The first code that is used is the All Orders Spectral Algorithm AORS2D [17] which is spectral in all three dimensions (R, Z, \( \phi \)). Here (R, Z, \( \phi \)) are cylindrical coordinates where ‘R’ lies in the equatorial plane of the tokamak, ‘Z’ is the vertical dimension, and ‘\( \phi \)’ is the toroidal angle. The code includes all cyclotron harmonics in the evaluation of the plasma conductivity [see Eq. (2)] and no assumption is made about the perpendicular wavelength (\( \lambda_{\perp} \)) relative to the ion gyroradius (\( \rho_i \)). The plasma response formulated in this manner leads to an integral relation and the resulting matrices that must be inverted are large, dense, non-symmetric, indefinite, and complex [17]. A second field solver TORIC [13, 18] is also used which employs a mixed spectral, finite element representation for the electric field in (\( \rho, \theta, \phi \)), where (\( \rho, \theta, \phi \)) are the usual pseudo-toroidal coordinates. The conductivity relation is truncated at second order in (\( \lambda_{\perp} / \rho_i \))^2 and at the second cyclotron harmonic. These
assumptions result in a closed form for the plasma response and a matrix system to invert that is sparse and banded with large dense blocks. Both the AORSA and TORIC matrix inversion algorithms take advantage of the resulting dense block structures by using the ScaLAPACK [19] library of parallelized linear algebra routines to efficiently invert their matrices.

3.2. Detection of Mode Converted ICRF Waves, Simulation Predictions, and Model Validation

Mode converted ICRF wave fields predicted by the full-wave solvers have been validated against experiment for plasmas where a high minority ion concentration of (H) and 3He is present [8, 13, 20, 21]. Although this is not the identical scheme described in Fig. 1, the high minority concentration leaves the cyclotron resonance well separated from the mode conversion layer. Also, the minority ion tail is relatively low energy owing to the high minority ion concentration; so that the Doppler broadened resonance does not overlap with the mode conversion layer [12]. Thus the effects of mode conversion can be studied somewhat separately from those of cyclotron damping in this case, which is not possible with the minority heating scheme (See Fig. 1).

Experimental measurements of mode converted ICRF waves have been made with a Phase Contrast Imaging Diagnostic (PCI) in the Alcator C-Mod tokamak for the scheme discussed above [20]. These measurements initially presented puzzling results because the short wavelength mode was detected on the low field side of the mode conversion layer and at a much longer wavelength (≈ 7 cm⁻¹) than what would be expected for IBW [20]. However, the PCI measurements were actually carried out in a three ion component plasma with parameters $B_0 = 5.8$ T, 33% H, 23% ³He, 21% D, $T_e \approx T_i \approx 1.5$ keV; where it was recognized that the detected mode would not be the expected IBW, but rather a longer wavelength electromagnetic ion cyclotron wave (ICW) [22], that is coupled to the fast wave through the presence of a poloidal magnetic field component. The correct dispersion relation for this case is shown in Fig. 2 [20] where it can be seen that indeed a short wavelength mode (the ICW) is excited to the low field side of the usual IBW mode conversion layer shown in Fig. 1. A massively parallel simulation of the ICW mode conversion scenario in C-Mod using the TORIC solver is shown in Fig. 3. The longer wavelength ICW are apparent in the simulation above and below the tokamak midplane and can be seen propagating back to the low field side of the mode conversion layer at $-2 \leq X(\text{cm}) \leq 0$.

![Figure 2: Dispersion relation for an ICW mode conversion scenario in Alcator C-Mod. Shown also is an overlay of the spatial location of the PCI laser chords.](image)

![Figure 3: TORIC simulation of the ICW mode conversion scenario for Alcator C-Mod using a 240 (N_r - radial) × 255 (N_m – poloidal) grid.](image)
where $X = R - R_{\text{axis}}$. Evidence of the shorter wavelength IBW can also be seen at the midplane. In Fig. 2, the fast wave is incoming from the low field side at $X \approx 20$ cm. The simulated mode converted wave fields from TORIC have also been used successfully in a synthetic diagnostic code to predict the detected signal of the PCI diagnostic [20, 21], lending further confidence in the capability of the full-wave solvers to accurately predict the detailed mode converted wave field structure. Referring to Fig. 4 it can be seen that the shapes of the measured and predicted PCI signals are in good agreement. The simulated PCI spectra in Fig. 4 include all of the toroidal modes coupled by the ICRF antenna in Alcator C-Mod.

Figure 4: Comparison of measured PCI signal with synthetic diagnostic code prediction for ICW mode conversion in Alcator C-Mod [reproduced from Y. Lin et al, Plasma Physics and Controlled Fusion 47, 1207 (2005)].

3.3. Predictions of ICW Mode Conversion in ITER and Scalability of Solvers

The potential of the mode converted ICW for localized generation of sheared flows has been

| Figure 5(a): AORSA simulation of mode converted ICW in ITER using a 350 ($k_R$) × 350 ($k_z$) mode resolution – full cross-section. |
| --- |
| Figure 5(b): AORSA simulation of mode converted ICW in ITER using a 350 ($k_R$) × 350 ($k_z$) mode resolution – blow up. |
investigated in present day devices [8] and for the ITER burning plasma device [23]. Fully resolved simulations of mode converted ICW have been obtained for ITER using the AORSA solver on the CRAY XT3 / XT4 Jaguar computer at Oak Ridge National Laboratory (see Fig. 5). The parameters used in these simulations were \( f_0 = 53 \) MHz, 20\% D, 20\% T, 30\% \(^{3}\)He, and \( n_e = 2.5 \times 10^{19} \) m\(^{-3}\). The results were obtained for a single toroidal mode and required 4096 processors for 1.5 hours of wall clock time. The poloidal field requirement for ICW excitation results in the characteristic off midplane feature of the ICW wave fields.

Accurate simulations of flow drive [23] will eventually require superposition of the mode converted wave fields excited by the entire toroidal mode spectrum of the ICRF antenna. In order to perform this type of simulation we have shown that the AORSA solver demonstrates excellent scaling with processor number up to 22,000 processors on the CRAY XT4 (see Figs. 6). A peak FLOP rate of 75 TF (TeraFlop) is achieved when the problem mode resolution is increased to 500 (\( k_R \)) \times 500 (\( k_Z \)), with the favorable scaling being a direct consequence of the heavy ScALAPACK utilization. These results indicate that it will be possible to consider hundreds of toroidal modes in future flow drive and current drive simulations for ITER.

![Figure 6: Scaling of wall clock time and ScALAPACK flop rate versus processor number for the ITER ICW mode conversion calculation shown in Fig. 5.](image)

4. Quasilinear Evolution of Nonthermal Ion Tails

As discussed in Section 2, a self-consistent simulation of ICRF heating requires a description of two different aspects of the wave-plasma interaction: (1) wave propagation and absorption in the plasma [see Eqs. (1) and (2)] and (2) the quasilinear response of the plasma to the wave heating. The long time scale response of the plasma distribution function \( f_0 \) can be obtained from a bounce-averaged, zero-orbit width Fokker-Planck equation of the form:
\[
\frac{\partial}{\partial t}(\lambda f_0) = \nabla_{u_i} \cdot \Gamma_{u_i}, \quad \text{with} \quad \nabla_{u_i} \cdot \Gamma_{u_i} = C(f_0) + Q(E, f_0).
\] (3a, 3b)

In these expressions: \(u_0\) is the velocity vector at the outside midplane; \(\lambda = \tau_b u_{(0)}\), with bounce time \(\tau_b\); and \(C\) and \(Q\) are, respectively, the bounce-averaged collision and quasilinear operators. This is a nonlinear problem in which the energetic ions generated by the waves can significantly alter the wave propagation and absorption in the plasma. Thus, we require an electromagnetic field solver that is valid for arbitrary non-Maxwellian distribution functions. The AORSA global-wave solver [15, 16, 17] has been combined with the CQL3D bounce-averaged Fokker-Planck code [24] and the Sigmad module for evaluation of the plasma response for arbitrary particle distributions [14] to simulate the quasilinear evolution of nonthermal ion distributions in ICRF heating. A reformulation of the quasilinear operator [15, 16] enables calculation of the velocity space diffusion coefficients directly from the global wave fields in differential form. To obtain self-consistency, AORSA and CQL3D are iteratively coupled (using the Python scripting language) in a stand-alone system in which both codes communicate and interact automatically on the same computing platform (the Cray XT3/XT4 Jaguar at ORNL).

In Figure 7, the combined self-consistent model is applied to minority hydrogen heating [25] in the Alcator C-Mod tokamak. Five iterative steps are shown in the self-consistent solution for 600 kW of fast wave power. This power induces a high energy tail on the hydrogen distribution function that is clearly evident in the figure. The tail is most extended in velocity space near the trapped-passing boundary where some of the ions have their turning points very close to the resonant surface and can, therefore, gain large amounts of energy. For the converged solution, the equivalent temperature is
about 72 keV at the radial location where the power deposition is maximum \(r/a = 0.45\), in good agreement with experimental measurements [25]. This calculation would not be possible without the massively parallel architectures required for the global-wave solver. For a spatial mesh of 256×256 cells in \((R, Z)\) and a velocity space mesh of 65×129 cells in \((u_\perp, u_\parallel)\), the solution in Fig. 7 required about 8 hours of wall clock time using 1024 processors on the Cray XT3/XT4. The need for high spectral resolution even in the case of ICRF heating at low minority concentration (Fig. 7) where mode conversion is weak can be seen upon examining the left circularly polarized electric field computed by AORSA in Fig. 8. Mode converted IBW can be seen clearly on the high field side near the midplane and mode converted ICW can be seen propagating back toward the low field side above the midplane. As discussed earlier, although very little power flows into mode converted waves during minority heating (< 10%), the presence of these short wavelength modes does alter the polarization of the incoming fast wave in the mode conversion region.

Although the minority cyclotron resonance layer passes through the plasma center in this case, the ICRF power dissipation is clearly peaked off-axis. This feature can be seen more prominently in Fig. 9 where we have plotted the 2D \((R, Z)\) minority power dissipation for the final (8th) iteration shown in Fig. 7. There is a clear peak in the 2D absorption along the resonance chord at about 0.07 m above the midplane. This location can be qualitatively correlated to the turning point of energetic ions that are undergoing so-called banana motion. These particles experience a decrease in their parallel (to \(B\)) velocity as they are heated near resonance in order to conserve their magnetic moment. Hence they spend more time at the turning point and experience a larger energy kick (i.e. more heating) from the ICRF wave at this point.

We have also used the 3D \((r, v_\perp, v_\parallel)\) nonthermal minority ion distribution function computed by AORSA-CQL3D (Fig. 7) in a synthetic diagnostic for passive and active neutral particle analysis [25].
This compact neutral particle analyzer (CNPA) diagnostic is used on C-Mod to measure the energy distribution of the minority hydrogen tail. A comparison of the predicted and measured neutral particle diagnostic signals is shown in Fig. 10. The spectra are normalized to the first CNPA data point for clarity and the error bars are based on counting statistics only. The agreement between the measured and simulated spectra is remarkably good [25]. It is thought that the failure of the simulated spectra to reproduce the negative sloping region in the passive data may be due to the omission of finite ion drift orbit effects in the AORSA-CQL3D simulation.

5. Conclusions and Future Work

It has been shown that access to massively parallel computing architectures has made it possible to resolve the disparate spatial scales associated with mode conversion of an ICRF fast wave to short wavelength ion Bernstein and ion cyclotron waves in the 2D geometry of a tokamak. This predictive capability has made it possible to accurately compute the wave fields needed to evolve a nonthermal distribution of minority ions via the solution of a 3D \((r, v_\perp, v_\parallel)\) Fokker Planck equation. The plasma response in the wave solvers was also re-evaluated using the new nonthermal particle distribution and the field solvers and Fokker Planck equation were iterated until self-consistency was achieved. Predictions for the mode converted wave fields were tested against experiment by constructing a synthetic diagnostic code to compare with measurements of mode converted waves made with a Phase Contrast Imaging diagnostic in the Alcator C-Mod tokamak. Predictions of the 3D \((r, v_\perp, v_\parallel)\) nonthermal ion distribution produced during minority ICRF heating were also tested against experiment by constructing a synthetic diagnostic code to compare with measurements of active and passive charge exchange spectra made in Alcator C-Mod.

In the future we plan to self-consistently couple the full-wave solvers to a Monte Carlo orbit code [26] in order to include the effects of finite ion drift orbits in the minority heating simulations. These effects can also be especially important when considering the interaction of ICRF waves with energetic neutral beam ions or energetic fusion alpha particles. Finally, we also plan to simulate the parasitic effects of RF sheaths that form near and away from ICRF antenna structures. Metal wall boundary conditions in the full-wave solvers will be modified to include sheath effects and time
domain simulations of the antenna – edge plasma will be carried out. It is expected that both of these future directions will require either sub-petaflop or petaflop computing capability.

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