Numerical Calculations of Wave-Plasma Interactions in Multi-dimensional Systems

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• How has the project responded to the 2002 PAC recommendations?
• How have super-computing resources enabled the achievement of the targeted scientific goals in the timeliest manner?
• What role have collaborative interactions within the project and also with other SciDAC activities played?
• Progress on achieving the scientific targets with respect to the stated timetable for deliverables which will end in June of 2004
• What is the vision/scientific roadmap for the next 3-year phase?
“PAC recommends that the overarching physics goals be more clearly articulated and that two or three targeted physics calculations be specified.”

Waves in magnetized plasmas exhibit many complex linear and non-linear behaviors having influence on science from fusion, to astrophysics, to Hawking radiation from black holes, to commercial plasma devices.

Therefore our first overarching goal is:

To obtain detailed, quantitative physics understanding of the wave-plasma processes at work in fusion experiments with an eye to applications in other fields.

In particular this project emphasizes those aspects of plasma wave theory which have heretofore been inaccessible because of extreme computation requirements arising from: high dimensionality, extreme separation of scale lengths, nonlinear coupling between waves and plasma.

Targeted physics calculations:

• Mode conversion of fast magnetosonic waves to short wavelength modes in realistic tokamak geometry

• Apply high resolution 2D full-wave codes to understand the spectral gap in lower hybrid current drive in tokamaks
“PAC recommends that the overarching physics goals be more clearly articulated and that two or three targeted physics calculations be specified.”

Waves also play a critical role in fusion as a practical tool to drive, control, and probe the plasma.

Therefore our second overarching goal is:

To develop and apply validated computational RF models, in conjunction with experiments, discharge simulations, transport models, stability models and the like, to obtain understanding of plasma phenomena, which may lie completely outside the domain of wave physics, and which ultimately will be required to make fusion devices function optimally.

Targeted physics calculations:

- Calculation of RF driven flows in tokamaks to determine their potential to influence turbulence, or to trigger or control transport barrier formation

- Calculate high harmonic fast wave propagation and absorption in NSTX in the presence of neutral beam injection with self-consistent plasma distribution
A beautiful story of science – 2D effects on mode conversion

Plasma waves have an unpleasant habit of changing their character in the middle of a non-uniform plasma

- On the right (low magnetic field) the ion cyclotron wave (fast wave) has long wave length and the IBW has short, imaginary wavelength (evanescent)
- In the center (near the ion-ion hybrid resonance) the modes interact
- On the left (high magnetic field) the fast wave has long wave length, the IBW has short wavelength, which must be resolved, but is well separated from the fast wave.
Understanding of a complicated phenomenon like plasma mode conversion builds on increasingly sophisticated theory, computation and experiment

We have progressed from:

- Simple, approximate, analytic theory (F.W. Perkins, 1977)
  - Provided valuable paradigms for mode conversion
  - Indicated several conversions were possible when poloidal field included
  - Did not give quantitative information for real 2D situations

To:

  - Verified analytic calculations with much more inclusive physics
  - Higher cyclotron harmonics, can treat short wavelengths

To:

- High-resolution solutions across the full plasma cross section (All Orders Spectral Algorithm AORSA2D, AORSA3D (JAEGER, 2002)
  - Includes arbitrary cyclotron harmonics
  - Very short wavelength structures – limited by computer size and speed, not formulation
  - Full solution across plasma, geometrical representation of antenna

First Fully Resolved 2D Calculations of Conversion of Fast Waves to Short Wavelength Modes Were Obtained Within Our SciDAC Project
Phase Contrast Imaging System

CO$_2$ laser ($\lambda = 10.6$ $\mu$m), expanded to width $\sim 15$ cm, in front of the E-port rf antenna, imaged to 12-channel HgCdTe detector.

Most sensitive to waves with vertically aligned wave fronts.

Laser intensity modulated so that rf signals can be detected at the beat frequency.

Wave $k_R$ obtained by Fourier transformation on signals from all 12 channels.

Experimental Observation

Contour Plot of Fourier Analyzed PCI Data

 PCI Signal Structure

Dispersion Curves near MC Region

Propagating towards the low field side.
Wavelength shorter than FW, but generally longer than IBW.
On the low field side of the H-³He hybrid layer.

Mode conversion in C-mod D(H) with large $n_\perp = 22$, small $B_p$

- With small poloidal field and large $n_\perp$, $k_x$ doesn’t dominate over $k_\parallel$, conversion occurs to both IBW and slow ion cyclotron wave
- Perkins’ 1D model neglected $n_\perp$
This process was modelled extensively with TORIC and compared to experiment.

The ICW solution is a weakly damped mode on the low field side of the hybrid layer.

The wave structure also appears in the $E_z$ contour of TORIC simulation.

This wave agrees with the PCI observation in all aspects, such as spatial location, and wavelength.

First experimental observation of MC ICW in tokamak plasmas

On-axis Mode Conversion

Experimental curve agrees with the TORIC simulation in the MC region $0 < r/a < 0.25$.

Total volume integrated MCEH power fraction $\Pi^{\text{MCEH}}$:
- Experiment: $\Pi^{\text{MCEH}} = 16\%$
- TORIC: $\Pi^{\text{MCEH}} = 14\%$

TORIC result also shows IBW is the primary MC wave for this on-axis MC.

$B_{\text{pol}}$, crucial for the existence of MC ICW, is small near axis.

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

Off-axis MC

- D-H hybrid layer at $r/a = 0.35$ (HFS)

- Good agreement of experiment curve and TORIC.

- Total $\square^{\text{MCEH}}$ in the MC region ($0.35 < r/a < 0.7$)
  - Experiment: 20%
  - TORIC: 18%


$f_{\text{rf}} = 80$ 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
**Surprise – conversion to electromagnetic ion-cyclotron waves can dominate conversion to electrostatic ion Bernstein waves**

- Understand spatial structure of measured ICW in Alcator C-mod, including up-down asymmetry
- Understand power flow and partition to either IBW or ICW
- Quantitative understanding of electron power deposition profile

*This can have practical importance*

- Bernstein waves damp on electrons, can drive current
- Ion cyclotron waves damp on bulk ions, can drive plasma flow† turbulence suppression
- Identification of promising flow drive experiment on Alcator C-mod
We know from experiments that RF can induce shear flows e.g.

**TFTR**

**Also can influence confinement (especially short wavelengths – IBW) e.g.**


Goals:
- Investigate fundamental nonlinear physics of wave induced momentum deposition and transport
- Use waves to probe physics of turbulence and transport barriers
- Perhaps develop practical methods to control turbulence and transport barriers in tokamaks/stellarators
Heuristic model for $E_r$ driven transport barrier – plasma flow plays a crucial role

- Pressure gradient
- Instability drives (radial profiles)
- Turbulent fluctuations
- Anomalous transport
- Reynolds stress

- Shear in $E_r$ breaks up turbulent eddies, reduces transport

- Bootstrap current

- Current profile

- Plasma flow $E_r$ profile

- Pressure driven flow

- Turbulence driven flow
Understanding/controlling turbulence requires understanding/controlling many non-linearly coupled processes.

RF (and other sources) can drive several of these processes, but RF driven flow gives a more “open loop” control of $E_r$. 
We plan to investigate basic RF flow drive physics in 2D (maybe 3D) and study various experimental scenarios for significant flow drive comparisons

- Within SciDAC we have already developed a number of key capabilities:
  - Full wave 2D solvers capable of resolving the short wavelength modes which effectively drive flows – AORSA, TORIC
  - Rigorous 2D theory of nonlinear RF force – post-processing module for AORSA
  - Wavelet analysis for analyzing k(x) and wave polarization
  - Simple force balance models for estimating order of magnitude of flows and shear

  *Physical Review Letters, 90 (2003)*

- We hope within this project to couple our RF force calculations to a more complete neoclassical/momentum balance model (e.g. NCLASS/FORCEBAL)

- In the longer term we would couple with stability codes to get accurate measures of the influence of RF driven flows on stabilization

- We see the need for a dynamical model, possibly a direct coupling with turbulence codes
  - Self-consistent treatment of ITB
  - Treat the transient effect on $E_r$ of polarization currents to trigger ITB

This constitutes an essential element of a comprehensive fusion simulation, and also is essential for understanding experiments of RF effects on turbulence and ITB formation
How have super-computing resource enabled the achievement of the targeted scientific goals in the timeliest manner?

We make significant use of the most powerful available supercomputers

- **NERSC, Seaborg**
  - Allocation $2.2 \times 10^6$ MPP (including reimbursements) – down from $3 \times 10^6$ MPP last year but managable
  - As preferred customer got free use of newly installed nodes for several months during breakin
  - Typical run $\sim 2048$ processors, obtain up to 0.8 GF/processor
  - Variability of efficiency remains an issue – randomly drops to $\sim 0.2$ GF/processor

- **ORNL, Cheetah**
  - Allocation variable – ORNL adopted Fusion as topical area but we compete with climate, materials and supernova for time
  - Typical run $\sim 16 – 48$ processors, 2 GF/processor

- **LINUX clusters at MIT and PPPL** – 48 node Beowulf with Myrinet(MIT)
We have used these computer resources effectively by continuing to parallelize and optimize our large codes and restructure algorithms (SSAP collaboration).

TORIC

- Out-of-core parallel linear solver enable fully resolved TORIC models for IBW and Ion Cyclotron Waves (ICW) using \((N_m=1023) \prod (N_r = 240)\) modes on 128 CPUs on Cheetah.
- Medium models with 255 modes can be solved in about 4hrs on a single Pentium 4.
- Original serial version limited to \((N_m=161) \prod (N_r = 240)\) modes required over 12hrs on NERSC CRAY.
- Today problem 500 times larger than previous maximum-feasible takes 4 times as much wall clock time – speedup x100
- Old serial computation would have required 6000 wall clock hours (250 days)

We have obtained converged solutions with \((N_m=1023) \prod (N_r = 480)\) modes.

This is sufficient to proceed with full wave treatment of lower hybrid physics.
We have used these computer resources effectively by continuing to parallelize and optimize our large codes and restructure algorithms (SSAP collaboration)

AORSA

- Code restructuring and optimization leads to 50X speedup in matrix construction in AORSA2D.
- Kronecker product formulation leads to 10X speedup in W-dot power calculation in AORSA2D.
- New AORSA formulation transforms from Fourier space back to configuration space – results in large reduction in matrix size and solution time
  - AORSA2D – speedup x3.7, matrix memory 1/2.5
  - AORSA3D – speedup x27, 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

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

3D example

Note:

Performance improves $\geq 27$

Efficiency drops/4
The high computational efficiency in FLOPS of the AORSA code has attracted a lot of attention.

More detailed writeup appears on successive pages.

The high efficiency is a direct result of optimization of ScaLAPAC on the dense linear solve that dominates AORSA performance.

NERSC brochure

This is us

New Computational and Scientific Results at NERSC

Science-of-Scale Applications Achieve Significant Results and up to 68% of Peak Performance on 10 Tflop/s IBM SP

April 2003

Initial results from NERSC’s 10 teraflop/s IBM SP supercomputer, which became available for general use in early March 2003, show scientific applications running at up to 68% of the system’s theoretical peak speed, compared with the 5–10% of peak performance typical for scientific applications running on massively parallel or cluster architectures. Performance results for four science-of-scale applications are shown in the following table:

<table>
<thead>
<tr>
<th>Project</th>
<th>Performance (% of peak)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electromagnetic Wave-Plasma Interactions</td>
<td>68%</td>
</tr>
<tr>
<td>Cosmic Microwave Background Data Analysis</td>
<td>50%</td>
</tr>
<tr>
<td>Terascale Simulations of Supernovae</td>
<td>44%</td>
</tr>
<tr>
<td>Quantum Chromodynamics at High Temperatures</td>
<td>13%</td>
</tr>
</tbody>
</table>

NERSC’s IBM SP, named “Seaborg,” is the most powerful computer in the United States available for unclassified research. Seaborg has 416 16-CPU IBM Power 3+ SMP nodes (a total of 6,656 processors) with a peak performance of 1.5 gigaflop/s per node. The system has the largest amount of aggregate memory available on any unclassified computer in the U.S.—7.8 terabytes—and a Global Parallel File System with 44 terabytes of storage.

The four computational science projects cited above are described in the following pages, along with their latest discoveries. Calculations for the wave-plasma interaction and cosmic microwave background projects would not have been possible on any unclassified American machine except Seaborg.
Powerful computers, improved physics/algorithim formulation, and code optimization allows studies that were absolutely impossible before SciDAC

- Routinely obtain fully resolved solutions for mode conversion in tokamak geometry (discussed previously)
- Beginning 2D studies in new physics domains with TORIC
  - Resolve shear Alfvén resonance at edge of tokamaks
  - Can treat lower hybrid waves in full-wave
- 3D calculations with AORSA3D for minority heating in LHD stellarator, and high harmonic fast wave heating for QPS compact stellarator
  - 2002 One full 3D calculation of LHD
  - 2003 Routine analysis of QPS developing viable heating scenarios, guiding machine design
  - Are investigating minority heating and high harmonic fast wave for QPS
What role have collaborative interactions within the project and also with other SciDAC activities played?

We are involved in 3 types of collaborations, each of which is essential.

Collaborations within the project

Collaborations with other SciDAC activities

Physics collaborations with people outside of the outside the project
Collaborations within the project

Ultimate success of each element of the project requires the interconnection of the various parts

Every institution in the project is involved in project collaborations with one or more other institution e.g.

- Full wave code common development and comparisons (ORNL AORSA-xD, MIT TORIC, PPPL METS)
- Preparation of TORIC and conductivity operator development of full wave lower hybrid studies (MIT, PPPL, ORNL computer science)
- Flow drive formulations, reduced spectral width methods, fast numerical wave diagnostics (Lodestar, ORNL)
- Interface of Fokker Planck (CQL3D) with full wave codes and generalized conductivity modules (CompX, PPPL, MIT, ORNL)
- Update of parallel gradient plasma response (generalized Z function) – incorporated in AORSA2D/3D, (Mission research, PPPL, ORNL)

We communicate with each other a lot

- Monthly (almost) conference calls
- Meeting at APS Nov. 2002, Orlando
- Many joint publications – see publication list at end
Collaborations with other SciDAC activities

Collaborative activities with SSAP project (D’Azevedo) continues to be productive and critical to success

- Massive parallelization and acceleration of AORSA 2D and 3D all orders wave codes
- Restructuring configuration space version of AORSA to eliminate boundary points
- Acceleration and parallelization of finite Larmor radius wave code TORIC
- Development of advanced field representations
- Acceleration of antenna modeling codes

There is potential for collaborations with other SciDAC activities, particularly the Fusion Grid, but none are presently under way at a significant level
Physics collaborations with people outside our project

- Experimental collaborations are playing a key role in code validation and application
  - Close collaboration has been established with RF experimentalists at Alcator C-mod
  - Computational tools developed through SciDAC are routinely used to understand RF experiments
  - Close collaboration established with NSTX RF experimental team
  - Initial tests of non-Maxwellian conductivity + METS fast ion distribution obtained from TRANSP simulation of NSTX: NBI+HHFW discharge

- New theory and computational collaborations will extend the applicability of codes
  - Monte Carlo calculation of ICRF induced plasma rotation – General Atomics
  - Global mode effects on antenna fields (TOPICA + EMIR3 codes) – Politecnico di Torino
  - Collaboration with U. Colorado on more general treatment of orbit integral
  - Johan Carlsson of TechX has received SBIR funding to work with us on PIC calculation of ICRF wave-particle interactions

- We are making a real effort to forge connections to other branches of the fusion program
  - Presentation at TTF on Nonlinear RF generation of sheared flows, Myra, Lodestar
  - We organized a special session at RF Topical Conf. to engage experimentalists and promote collaborations
Progress on achieving the scientific targets with respect to the stated timetable for deliverables – Our goals were:

• Complete analysis of 2D mode conversion in the light ion minority case and develop an understanding of the various roles on ion Bernstein waves and slow ion cyclotron waves, their dependence on poloidal field and other plasma parameters and the possibilities for direct ion heating by this method
  |-- On schedule – 2 Physical Review Letters

• Understanding of role of quantum chaos effects on filling spectral gap in lower hybrid current drive.
  |-- On schedule
  -- Extension of TORIC to LH wavelength resolution and speed
  -- Modified dielectric tensor elements valid in LH range of frequencies $\omega_{ci} << \omega << \omega_{ce}$
  -- Solutions obtained for LHRF wave-fields in the fast electromagnetic mode

• Explore modifications to wave dynamics in plasmas with significant non-thermal populations and two dimensional equilibrium inhomogeneities
  |-- Almost on schedule (loss of Remi Dumont)

• Implement alternative field representations in 1D to study ways to do adaptive gridding in all orders codes
  |-- Good progress – spline basis, wavelet basis and wavelet based conductivity

• Development of advanced matrix solvers (iteration pre-conditioning, out-of-core, fast moment methods…)
  |-- Little emphasis, concentrated on other tasks – parallelization of TORIC, configuration space transformation of AORSA, Kroneker product methods in W-dot calculation…
Progress on non-Maxwellian conductivity operator

- Finished implementation, optimization and benchmarking of parallel 1D METS code with general equilibrium velocity distributions included in the dielectric operator
- Utilized code to assess effects on non-Maxwellian distributions in various regimes, including:
  
  Combined High Harmonic Fast Wave Heating with Deuterium Neutral Beam Injection in NSTX
  
  - Beam anisotropy due to injection angle can modify fast ion absorption by a factor of 2
  
  D-T Mode conversion in TFTR with Tritium Neutral Beam Injection
  
  - Tritium ion absorption profile is much narrower with slowing down distribution than with equivalent Maxwellian

  Minority $^3$He heating of D-T plasmas in ITER with co-resonant fusion alphas
  
  - Power partitioning between alphas and the minority $^3$He is sensitive to the equilibrium velocity distributions and that coupling with a Fokker-Planck module is required for accurate analysis
HHFW + NBI on NSTX: Wave absorption is strongly modified by inclusion of anisotropic fast ion distributions

Electron absorption

- Without beam: 70 % (per pass)
- Isotropic beam: 24 %
- Anisotropic beam: 44%

Deuterium beam ion absorption

- Without beam: 0 % (per pass)
- Isotropic beam: 70 %
- Anisotropic beam: 35%

- Isotropically slowing down and equivalent Maxwellian in agreement
- Significantly less fast ion absorption predicted in the case of tangential injection
  - implies less degradation of HHFW-CD efficiency

One of our targeted physics calculations is study of high harmonic fast wave propagation and absorption in NSTX in the presence of neutral beam injection with self-consistent plasma distribution.

Goal: To understand and optimize compatibility of HHFW heating and CD with NBI
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 wavelet field representation

- Fourier basis set implies a uniform grid
- Have investigated Gabor transform (related to Morlet wavelet) Gaussian Window \( X \) Fourier as a basis set instead … each window can have uniformly spaced points of different density.
- 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)
Progress on rapid data analysis and visualization using wavelets

- New modified wavelet technique has been developed for diagnosing the rf wave solutions produced by AORSA and TORIC
  - Want to extract local dispersion $k(x)$, amplitude and polarization
- Example DIII-D D(H) mode conversion reference case
  - RF fields from AORSA1D with poloidal field chosen to simulate $E(x)$ above the midplane

Contour plot of $k$-wavelet power density
- Color palette indicates linear vs circular wave polarization
- Working to extend to 2D
So, where will we stand by June 2004?

We will have made significant physics advances in:

- Understanding wave behavior in 2D and 3D, particularly in mode conversion
- Understanding RF driven plasma flows and defining experiments to test effects on turbulence and transport barriers
- Resolving questions of lower hybrid coupling, focusing, diffraction and ray chaos
- Understanding and optimization of HHFW propagation in NSTX and compatibility with NBI

These advances will be based on the development of new supercomputing tools:

- Computationally efficient, benchmarked, 1D, 2D and 3D full-wave solvers in the FLR and all orders models
- Improved modules for plasma wave conductivity including non-Maxwellian distributions, and improved treatment of non-local parallel particle response
- Integrated, self-consistent solution for non-Maxwellian distributions from CQL3D and TRANSP Fokker Planck models

We will have laid a basis for future developments:

- Efficiency gains in wave solution through advanced field representations, adaptive gridding, iterative solutions
- Advanced solution of Fokker Planck equation using orbit methods
What is the vision/scientific roadmap for the next 3-year phase

- Extension of work under this SciDAC
  - We will have only scratched the surface of the basic RF physics studies and physics extensions possible with the tools developed
  - There will be many opportunities for code improvements/speedup and improved coupling between components

- Establishing connection to other disciplines setting the stage for an integrated fusion simulation
  - we have many ideas for coupling RF effects to other critical areas:
    - current drive interactions with MHD (discussions with S. Jardin)
    - fast particle effects on plasma rotation (discussions with V. Chan)
    - providing source terms for neoclassical modeling e.g. NCLASS (discussions with W. Houlberg)
    - flow drive interaction with turbulence and internal transport barriers (presentation at TTF)

- Preparation for burning plasma experiment
  - Any burning plasma experiment, including ITER, will be a driven system \((Q \leq 10)\) under most or all of its operation
  - We are already being called upon to validate and optimize the heating/current drive scenarios and RF system designs,
  - Specific tasks will include:
    - Improving physics and self-consistency of energetic particle effects, validation by experimental comparison
    - Integration with transport and time dependent simulation models to develop scenarios
    - Applying the RF codes by participating in the international ITPA activities

- A critical issue for RF applications is to come to some sort of understanding of edge/antenna interactions – To make meaningful progress will require an extensive collaboration with the edge modeling community and experiment/technology