Integrated modeling of wave-plasma interactions in fusion systems: A project on Scientific Discovery through Advanced Computation

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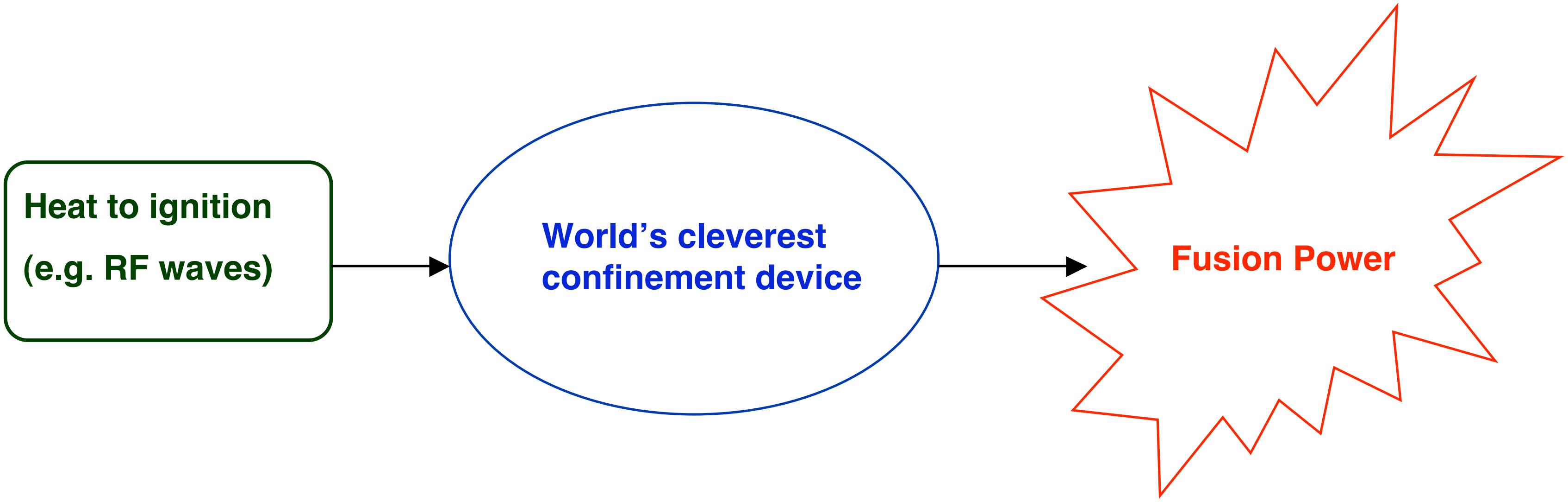
Workshop on theory based modeling and integrated simulation of burning plasmas

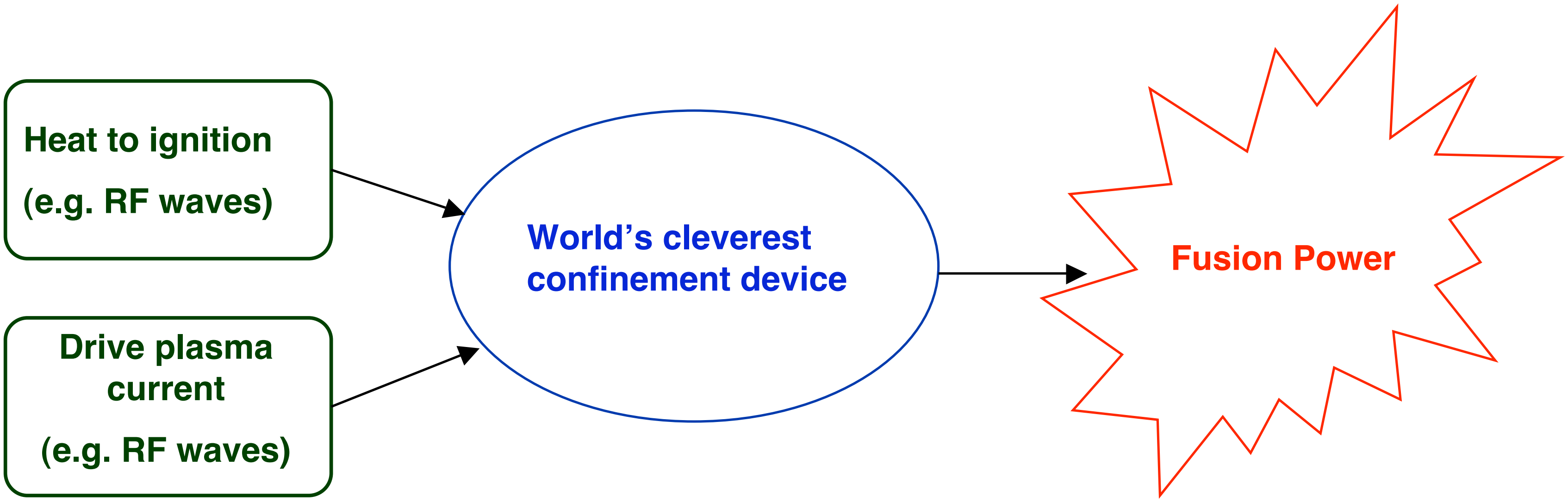
Dec. 15-17, 2003

Kyoto, Japan

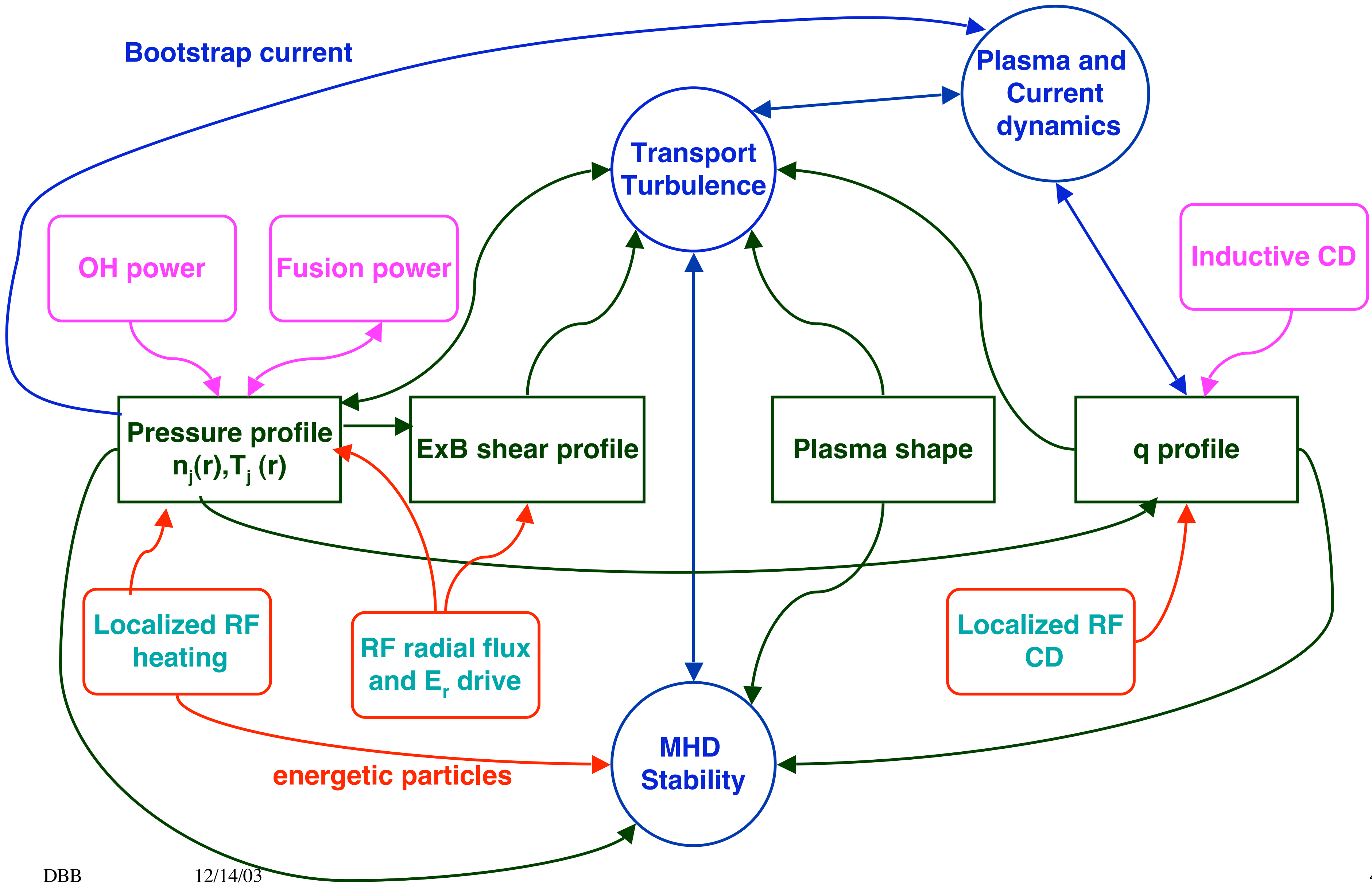
A primitive view of RF heating in fusion



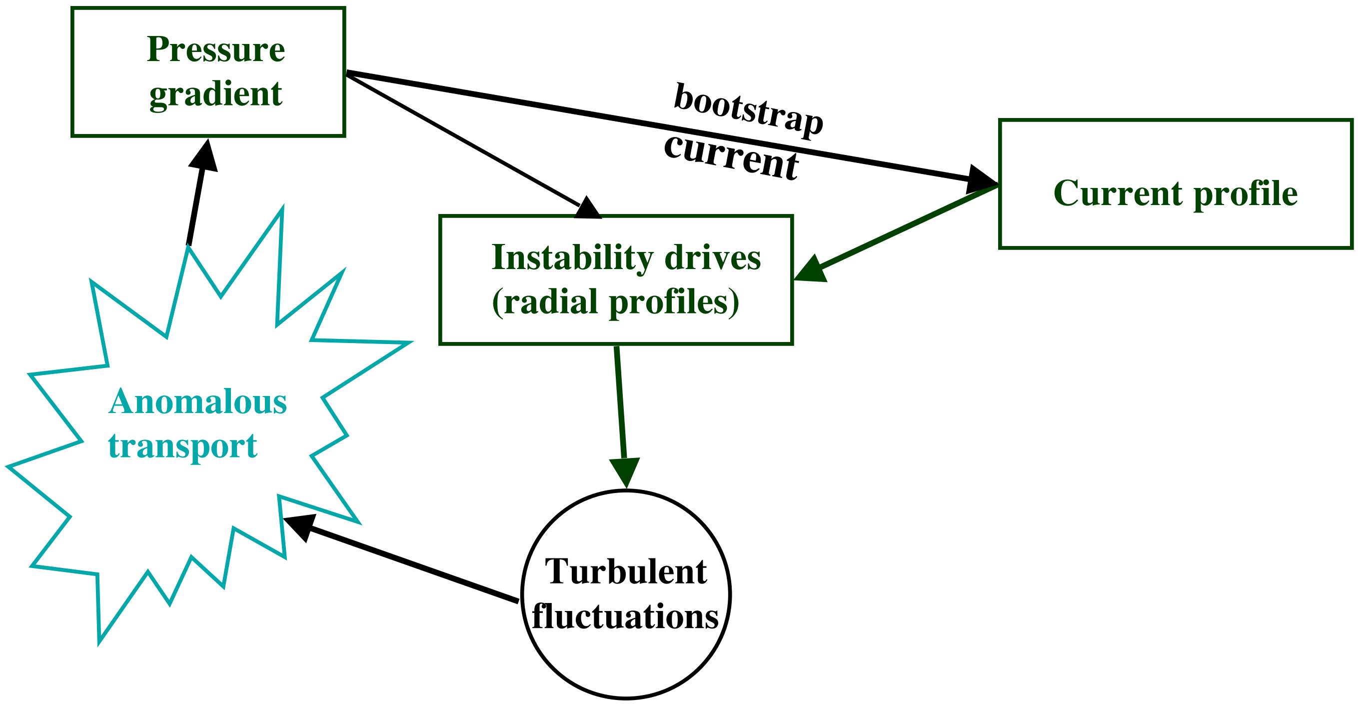
A slightly less primitive view of RF heating in fusion



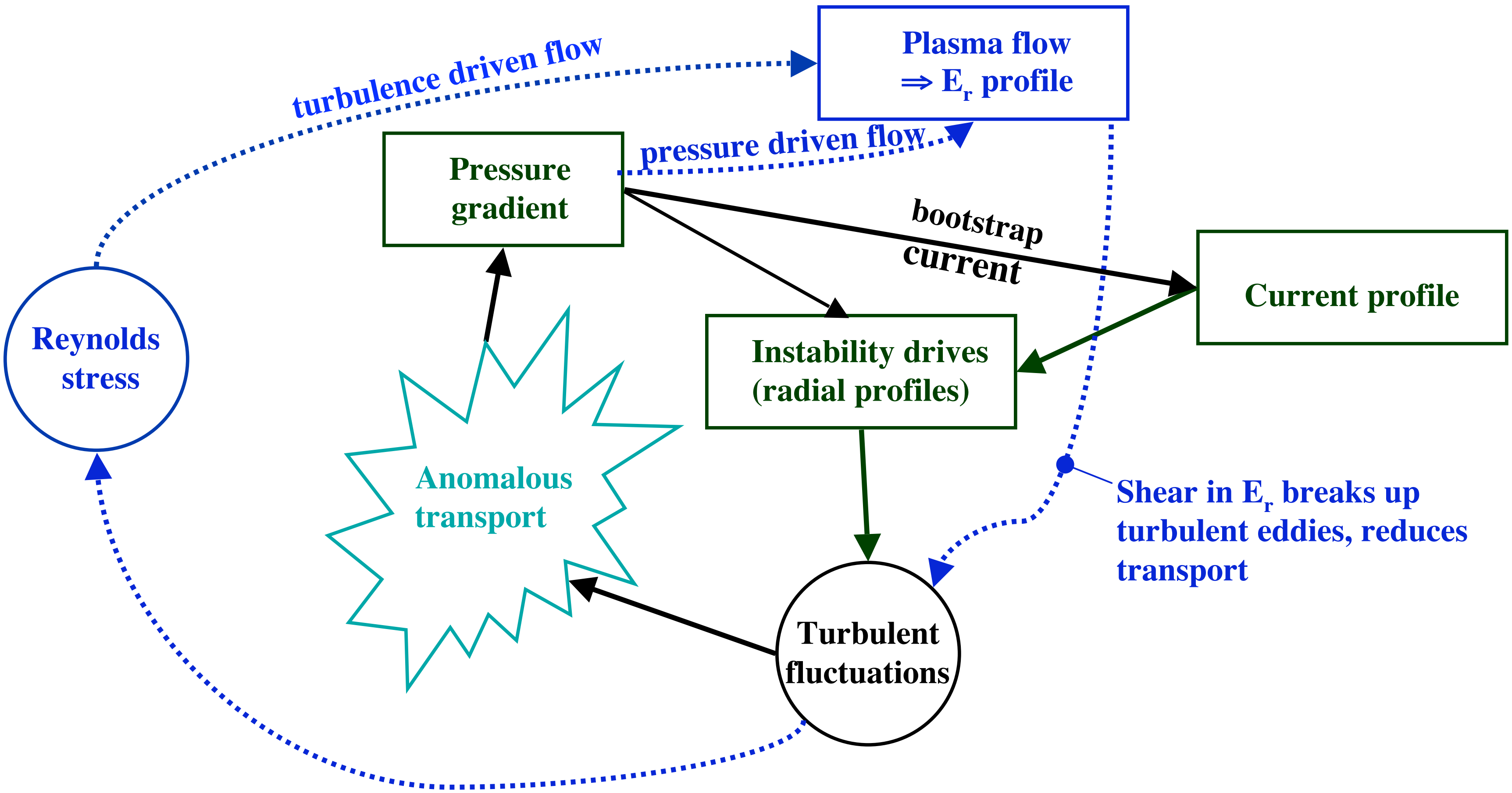
A more modern view



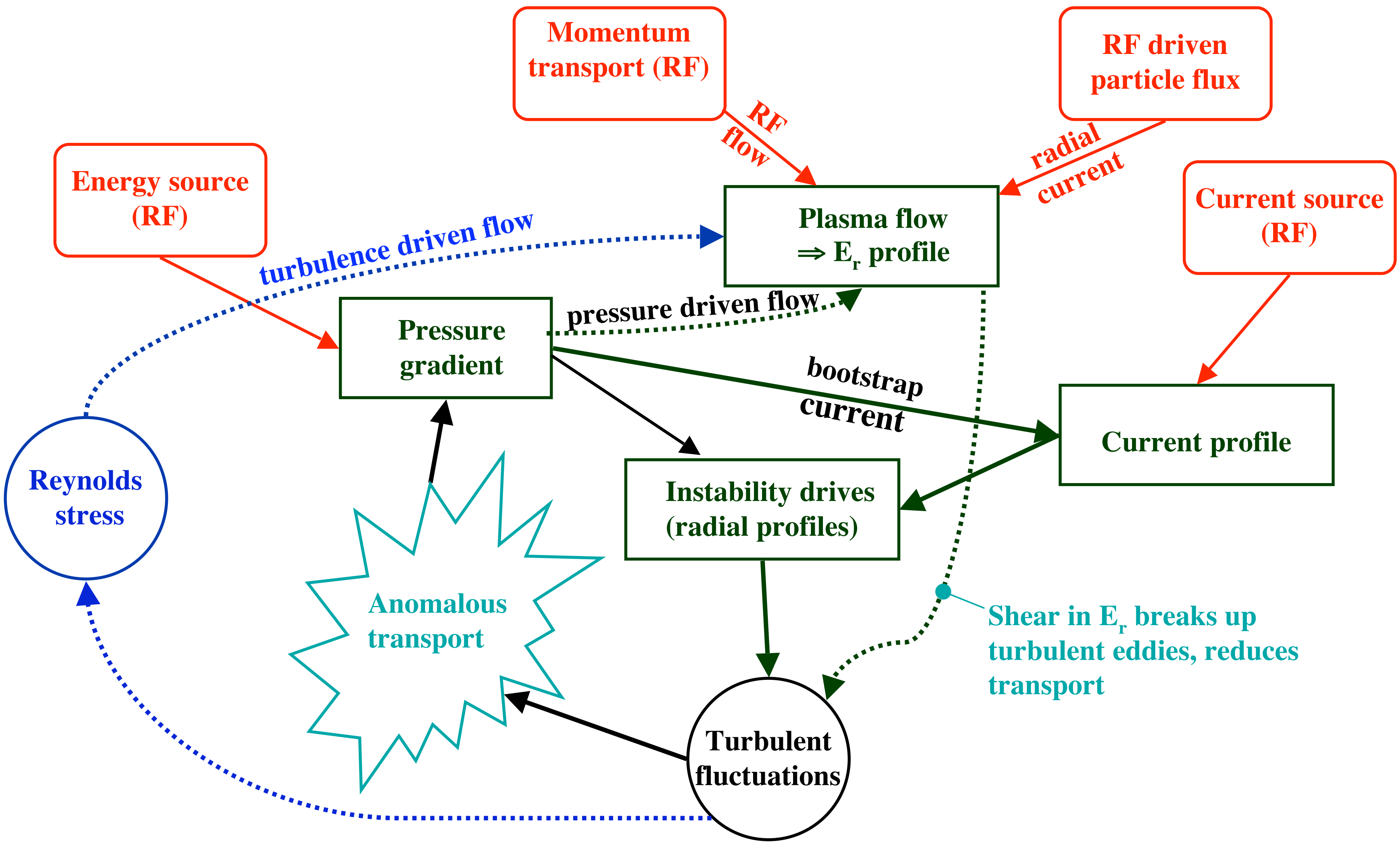
Transport is dominated by several, tightly coupled feedback loops



Heuristic model for E_r driven transport barrier – plasma flow adds yet another coupled feedback loop

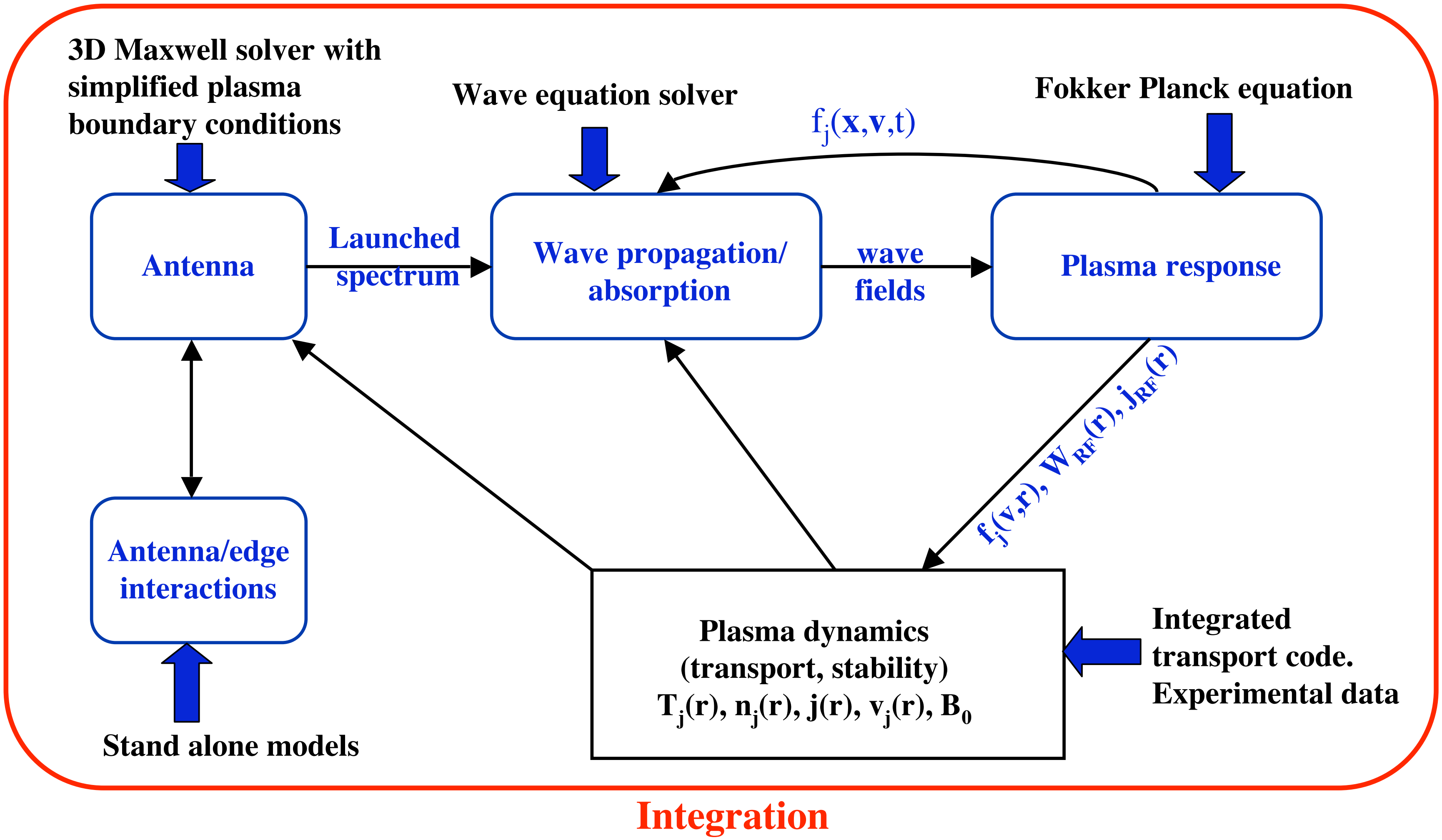


Success in fusion requires **understanding** and **controlling** many non-linearly coupled processes



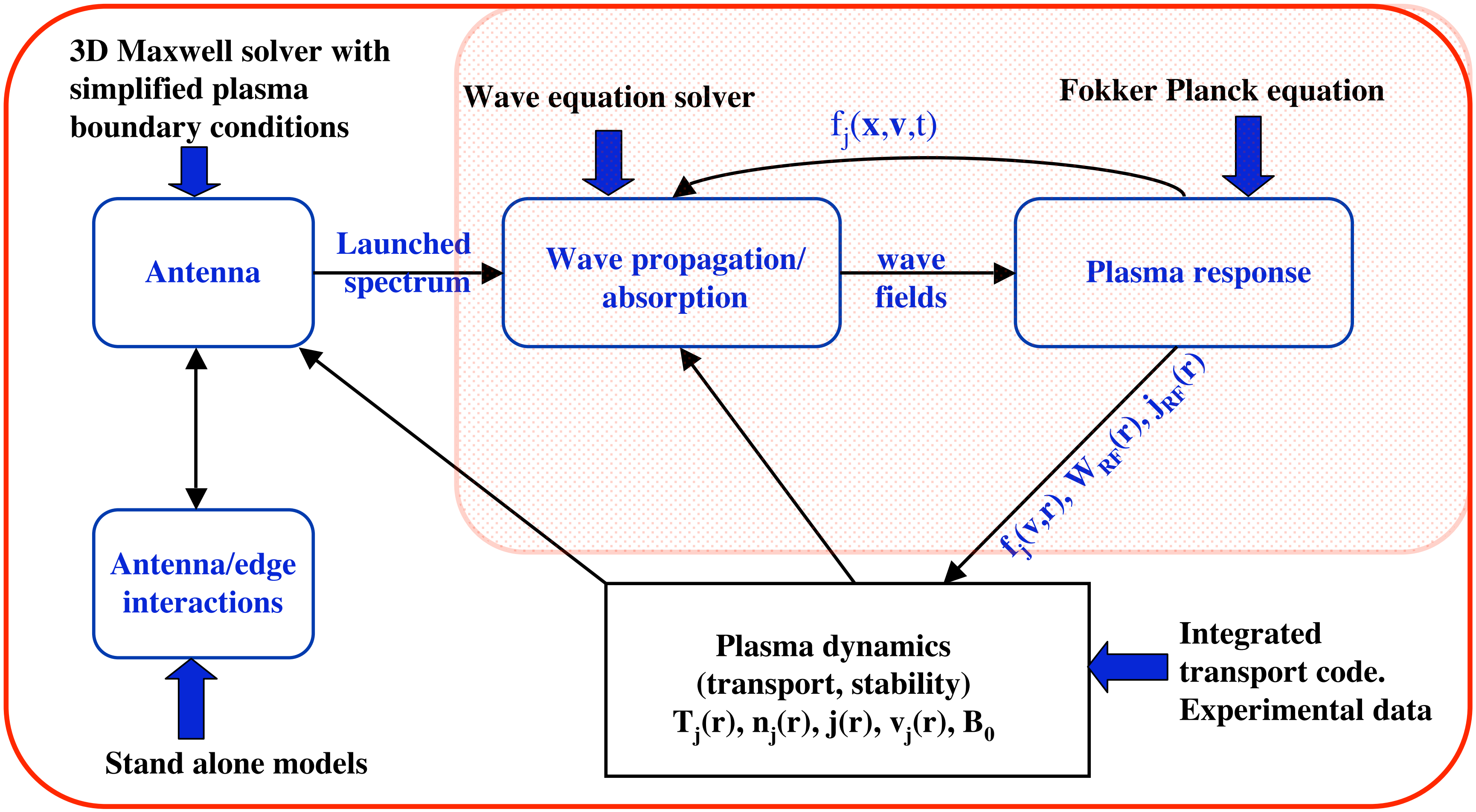
RF (and other sources) can drive several of these processes, and perhaps give an "open loop" control.

Integrated RF modeling requires a number of interconnected components



Our goal is to obtain quantitatively accurate, predictive understanding of wave processes important for heating, current drive, and stability and transport applications

Integrated RF modeling requires a number of interconnected components



Integration

Our goal is to obtain quantitatively accurate, predictive understanding of wave processes important for heating, current drive, and stability and transport applications

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

- **Separation of time scales – wave period 1/ω << time of equilibrium variation τ**
- **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**

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

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

What advances were needed?

- Adequate description of parallel plasma response – beyond the Z function, generalized Z function of Smithe and Colestock
- Higher harmonics – $\omega > 2\ \Omega_{ci}$ – eliminated by 2nd order expansion in $k_\perp\rho$
- Treatment of very short wavelength modes (e.g. IBW) – restricted by 2nd order expansion in $k_\perp\rho$
- Non-Maxwellian equilibrium distributions – general distribution in RF conductivity for wave codes, coupling to Fokker-Planck solvers for self consistency
- 3D – stellarators

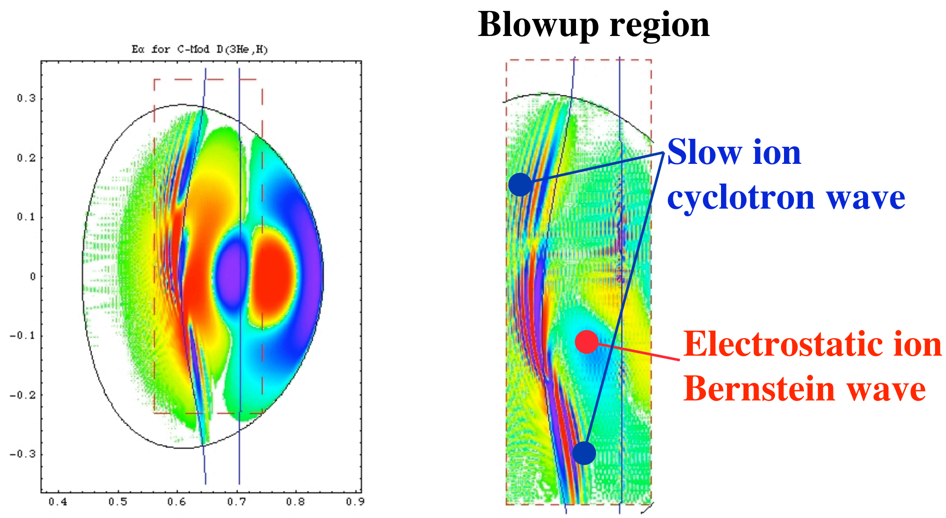
- Computer power/code acceleration
  - Much larger memory and/or out of core techniques to allow higher resolution
  - Much higher processing speed/massive parallelization to allow improved physics and higher resolution

We are advancing four wave solver codes within our project for various physics applications

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

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

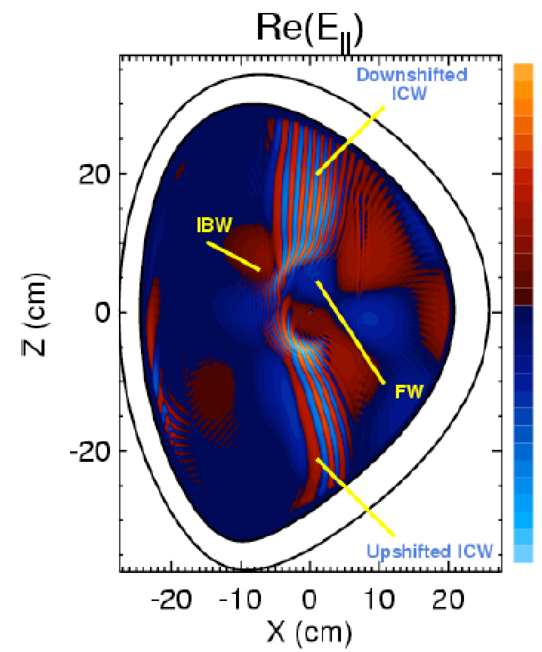
  - **Includes all cyclotron harmonics**
  - **No approximation of small particle gyro radius ρ compared to wavelength λ**
  - **Produces huge, dense, non-symmetric, indefinite, complex matrices**



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

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

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

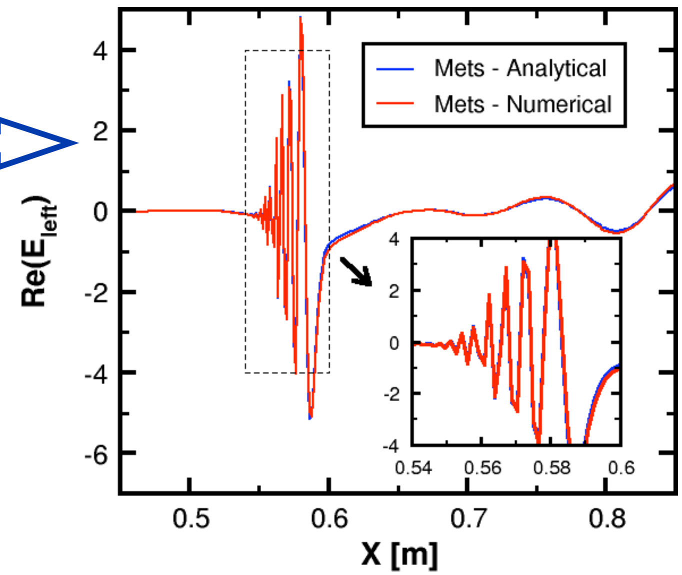


We are advancing four wave solver codes within our project

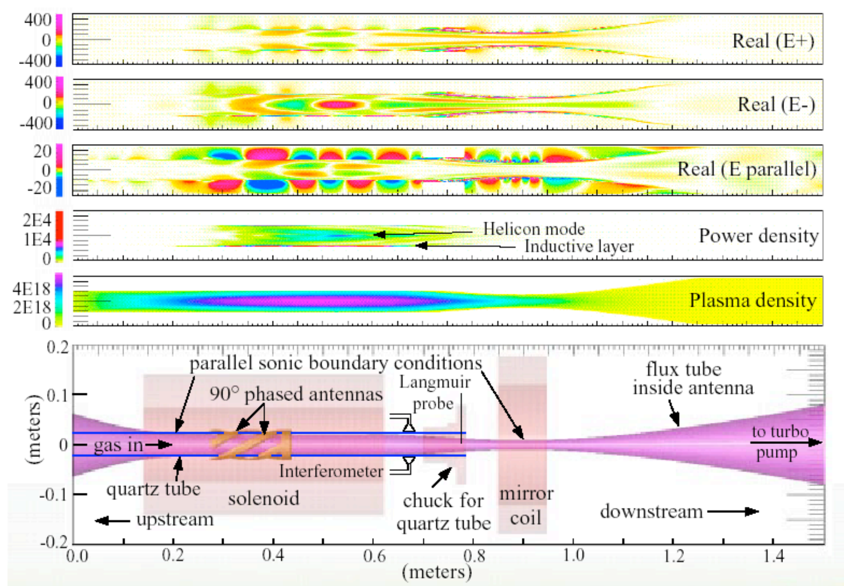
- **METS-1D (D. N. Smithe/Phillips) → All orders, fully spectral code in 1D**

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

  - **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**



- **EMIR 3**
  - **Finite difference**
  - **Adapted for open field line systems: plasma propulsion, simplified stellarator geometry**
  - **Iterates with source/transport model**



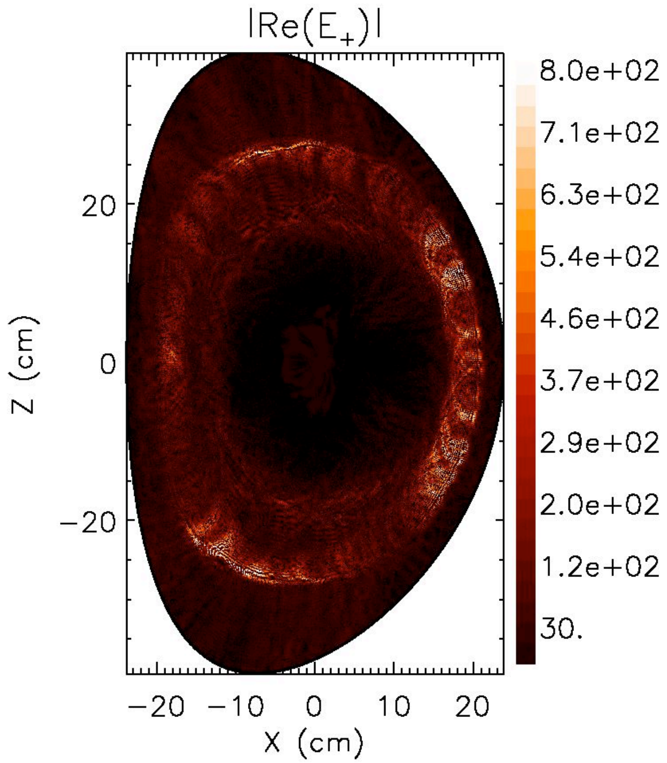
Our efforts at code parallelization and optimization have broadened the range of possible physics studies, and begins to allow coupling of full-wave to other codes

TORIC code

- **Original serial version limited to (N_m=161) × (N_r = 240) modes required over 12hrs on NERSC CRAY. ⇒ One-time event, solution unconverged**
- **Out-of-core parallel linear solver enable fully resolved TORIC models for IBW and Ion Cyclotron Waves (ICW) using (N_m=1023) × (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.**
- **Today problem 1000 times larger than previous maximum-feasible can be done on local MIT cluster**
- **Old serial computation would have required 12,000 wall clock hours (500 days) on Cray**

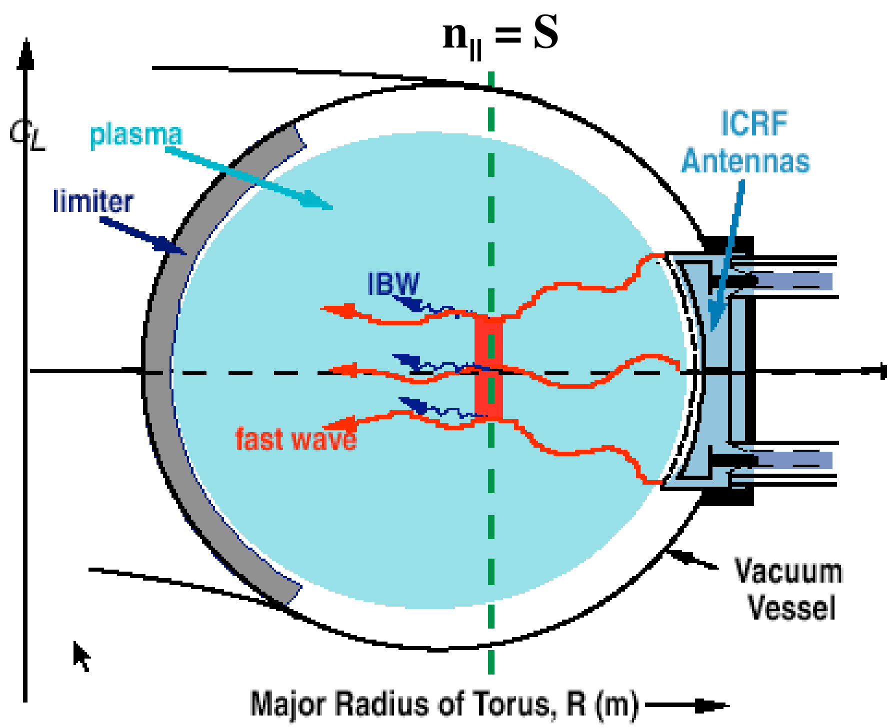
We have obtained converged solutions with (N_m=1023) × (N_r = 1000) modes.

This is sufficient to proceed with full wave treatment of lower hybrid physics without resorting to geometrical optics approximation

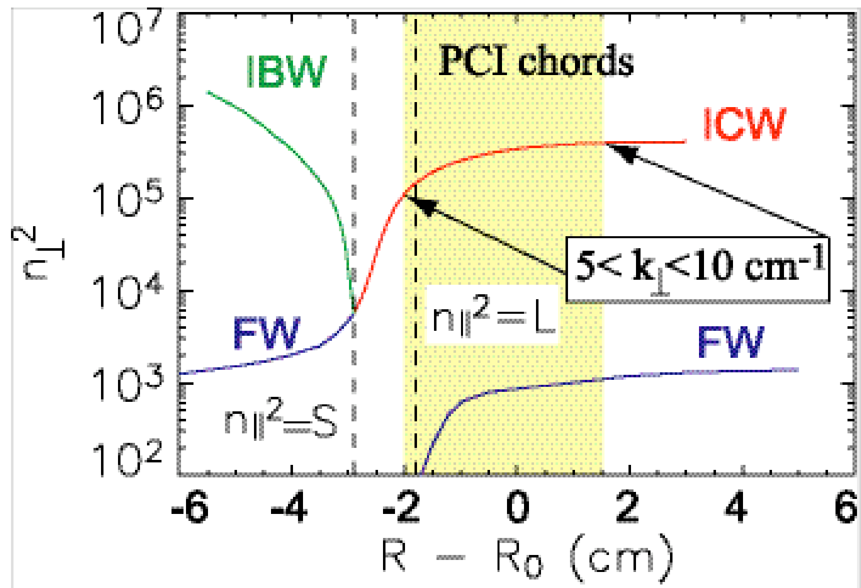


Experimental comparison – 2D effects on mode conversion

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



Dispersion Curves near MC Region



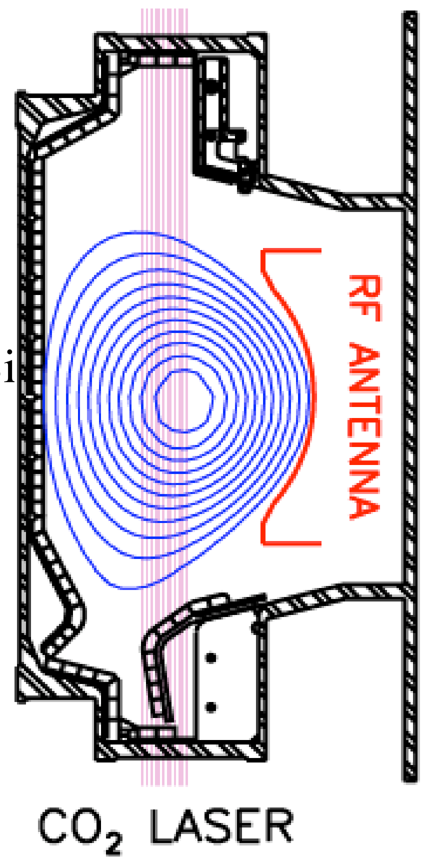
- On the right (low magnetic field) the launched fast wave has long wave length
- In the center (near the ion-ion hybrid resonance) the modes interact
- On the left (high magnetic field) the fast wave has long wave length, the IBW has short wavelength, which must be resolved, but is well separated from the fast wave.
- However another mode, the slow ion cyclotron wave, also exists on the right

First experimental observation of mode conversion to the ion-cyclotron wave in a tokamak plasma

E. Nelson-Melby *et al*, Phys. Rev. Letter, 90 (15) 155004 (2003)

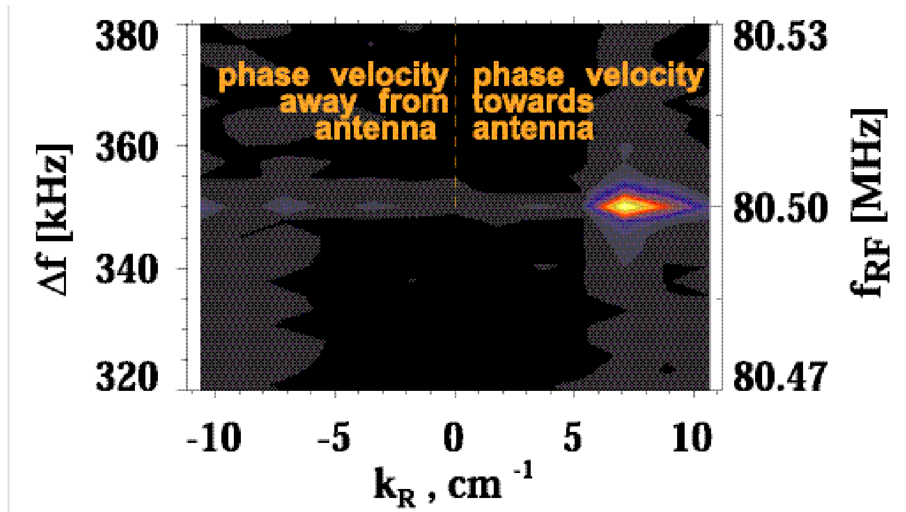
Y. Lin *et al* invited paper, APS 2003, Alberqueque

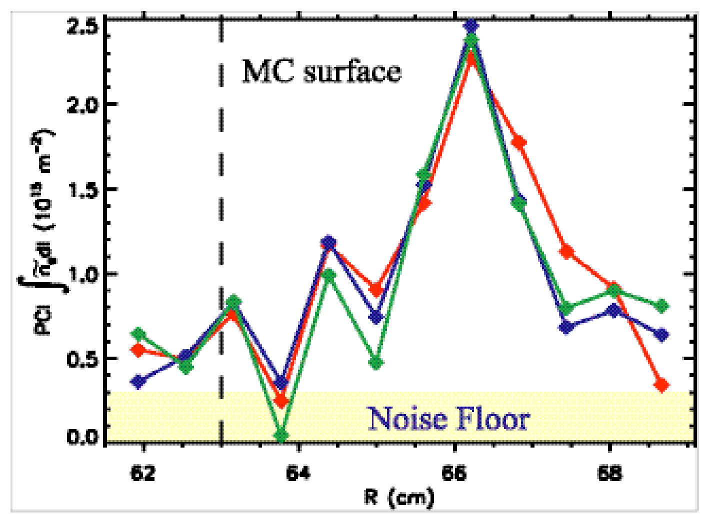
Phase contrast imaging system on Alcator C-Mod



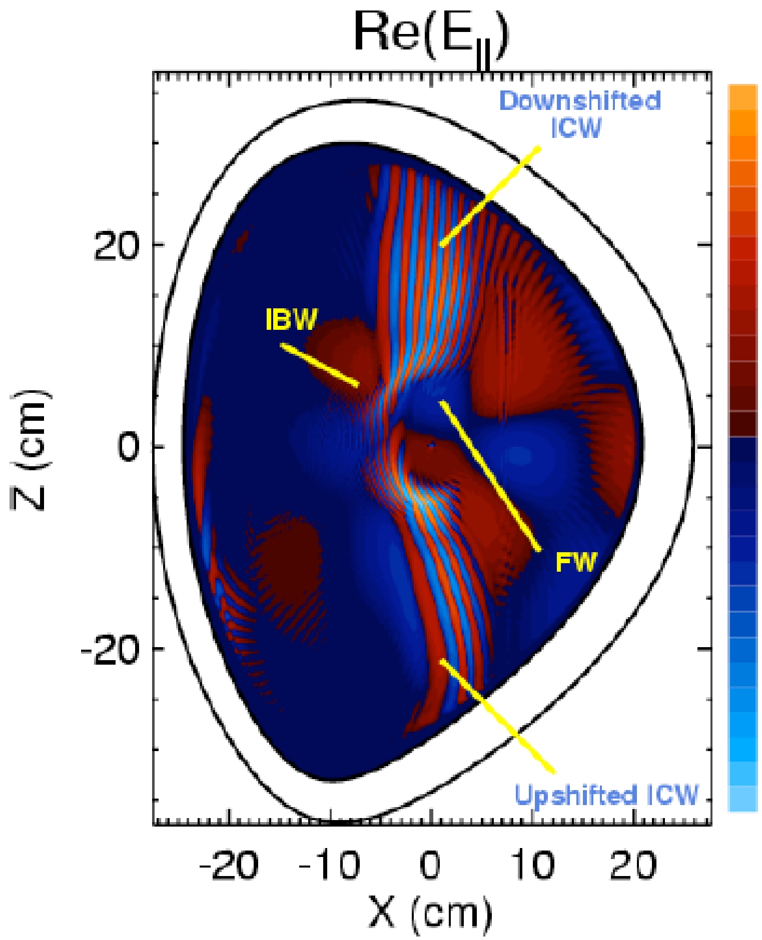
PCI Si

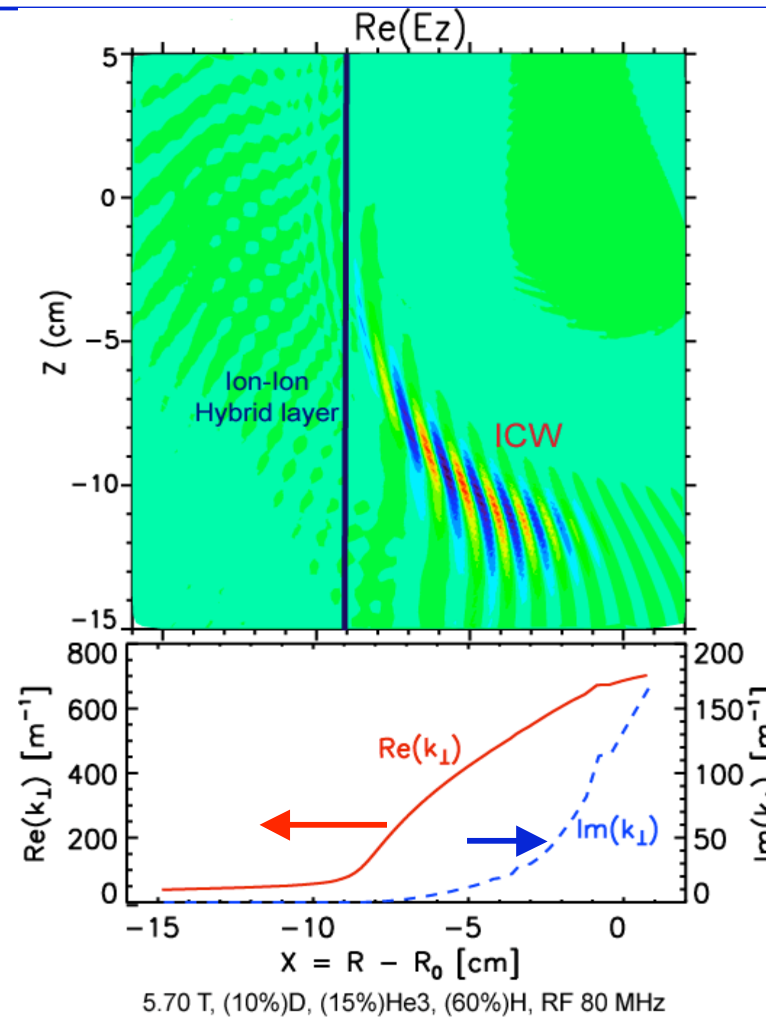
Contour Plot of Fourier Analyzed PCI Data





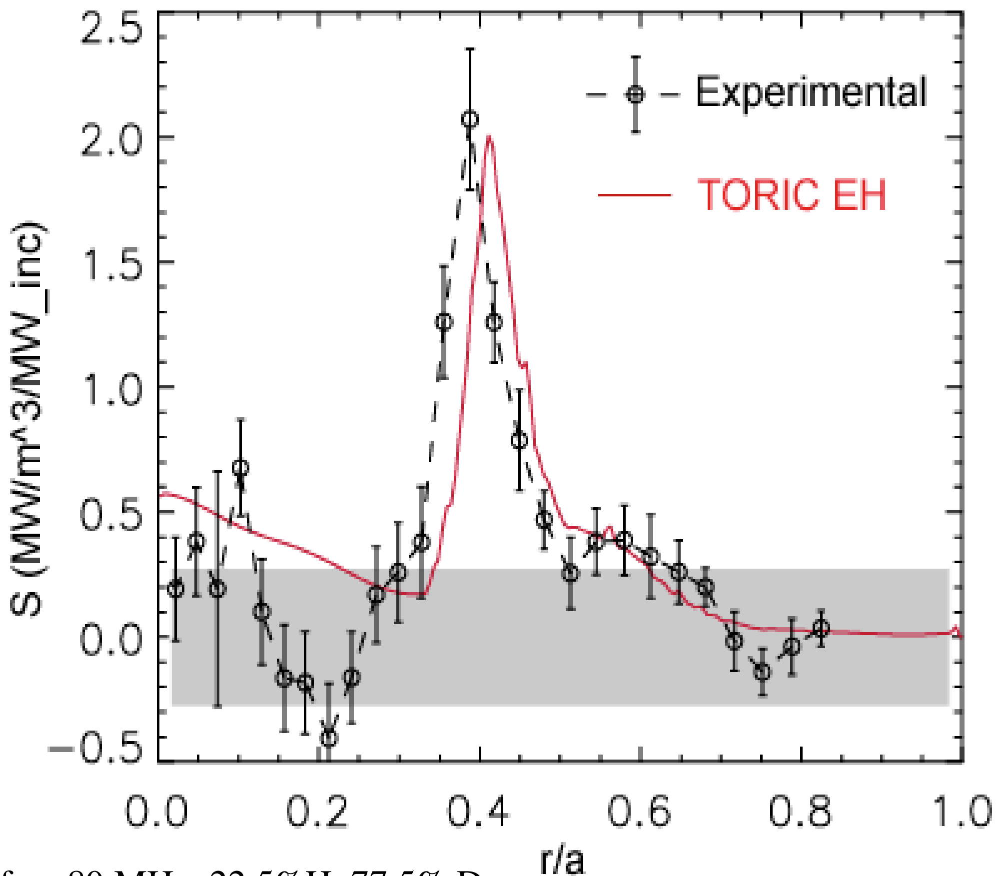
This process was modelled extensively with TORIC and compared to experiment





- 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 in all aspects, such as spatial location, and wavelength.

Off-axis Mode Conversion in C-Mod



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*: Invited paper, 15th Topical Conf. On RF in Plasmas

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

Note:

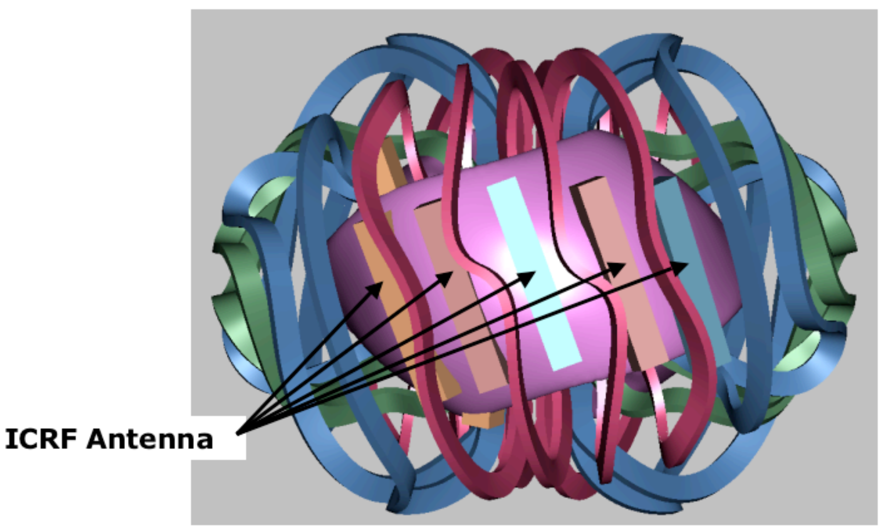
Performance improves × 27 ⇒ (Total CPU time)

Efficiency drops/4 ⇒ (Flops/processor)

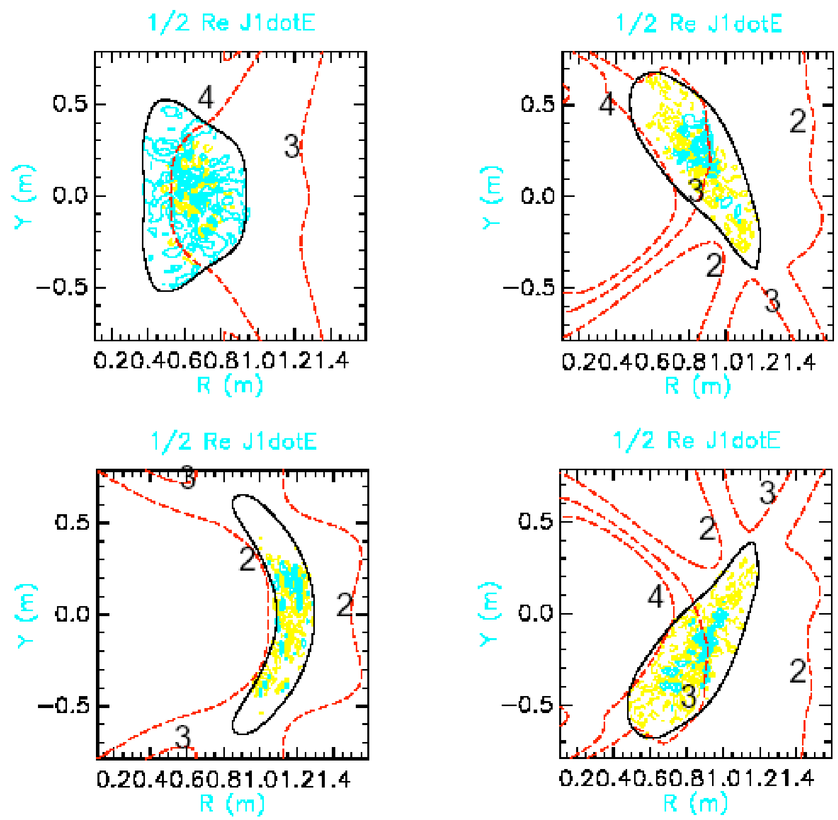
	Fourier space	Configuration space
Number of equations	248,832	39,492
Matrix size	990 Gbytes	25 GBytes
Time to load matrix	1.2 min	7.1 min
Matrix solve (ScaLAPACK	344 min	3.5 min
Fourier transform	9.5 min	0.04 min
Total CPU time	358 min	13.4 min
Flops/processor	1.1 Gflops	0.25 Gflops

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



A conductivty module allowing general plasma distributions has been developed – all orders, all cyclotron harmonics, shared by all wave solvers

Conductivity tensor

$$\overline{\overline{\mathbf{K}}}(x, k_x) = \overline{\overline{\mathbf{1}}} + \left(1 - i\frac{\partial}{\partial k_{2,x}} \cdot \frac{\partial}{\partial x}\right)\overline{\overline{\mathbf{W}}}(x, k_{1,x}, k_{2,x})\Big|_{k_{1,x}=k_{2,x}=k_x}$$

$$\overline{\overline{\mathbf{W}}}(x, \mathbf{k}_1, \mathbf{k}_2) = \frac{\omega_p^2}{\omega^2}\sum_{n=-\infty}^{\infty}\exp(in(\beta_1 - \beta_2))\overline{\overline{\mathbf{C}}}^{-1}(\beta_1) \cdot \overline{\overline{\mathbf{\Theta}}}_n \cdot \overline{\overline{\mathbf{C}}}(\beta_2)$$

Rotation matrices (Lab frame - local magnetic frame)

kernel in Stix frame

$$\overline{\overline{\mathbf{\Theta}}}_n(x, \mathbf{k}_1, \mathbf{k}_2) \equiv \int_0^{\infty} d\tau \int_0^{\infty} dv_{\|} e^{\left(i(\omega\tau - n\theta(\tau) - k_{\|,1}v_{\|}\tau)\right)} \int_{-\infty}^{\infty} dv_{\perp}\ \overline{\overline{\mathbf{w}}}(x, \mathbf{v}, \mathbf{k}_1, \mathbf{k}_2)$$

General expression for **w** (arbitrary distribution)

$$\overline{\overline{\mathbf{w}}} \equiv \begin{bmatrix} \frac{v_\perp}{\sqrt{2}}J_{n+1}(\xi_2) \\ \frac{v_\perp}{\sqrt{2}}J_{n-1}(\xi_2) \\ v_{\|}J_n(\xi_2) \end{bmatrix} \begin{bmatrix} \frac{\hat{L}f_0}{\sqrt{2}}J_{n+1}(\xi_1) & \frac{\hat{L}f_0}{\sqrt{2}}J_{n-1}(\xi_1) & \hat{L}_n f_0 J_n(\xi_1) \end{bmatrix}$$

Differential operators

$$\begin{cases} \hat{L}f_0 \equiv \left(1 - \frac{k_{\|}v_{\|}}{\omega}\right)\frac{\partial f_0}{\partial v_\perp} + \frac{k_{\|}v_\perp}{\omega}\frac{\partial f_0}{\partial v_{\|}} \\ \hat{L}_n f_0 \equiv \frac{n\Omega_0}{\omega}\frac{\partial f_0}{\partial v_\perp} + \left(1 - \frac{n\Omega_0}{\omega}\right)\frac{\partial f_0}{\partial v_{\|}} \end{cases}$$

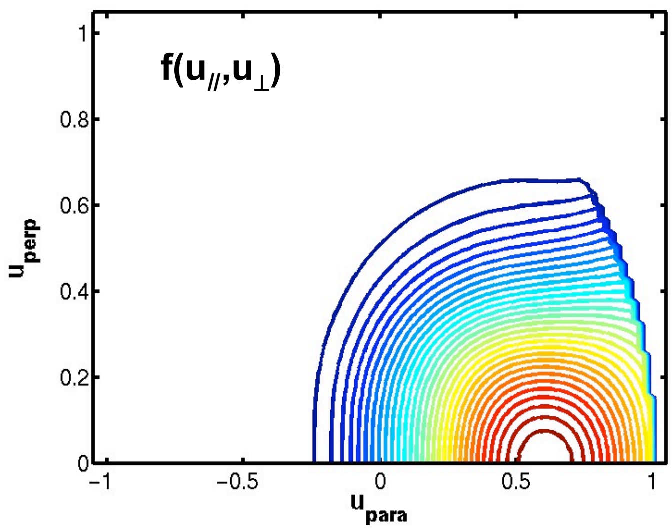
Tremendous increase of computational requirements

Non-Maxwellian conductivity has been tested in METS-1D comparing Maxwellian, isotropic beam, and anisotropic beam models

HHFW + NBI on NSTX

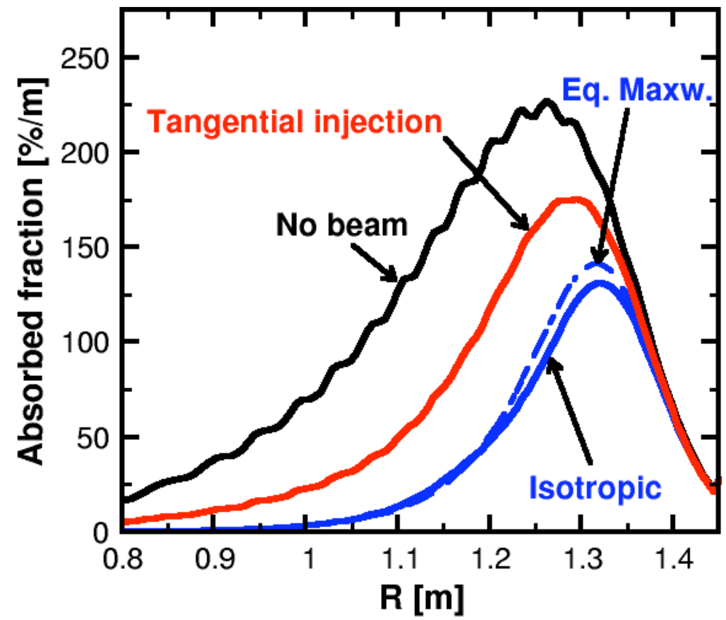
$$f(u,\mu) = \sum_{l=0}^{\infty} a_l(u) P_l(\mu),$$

Legendre polynomials



Tangential injection

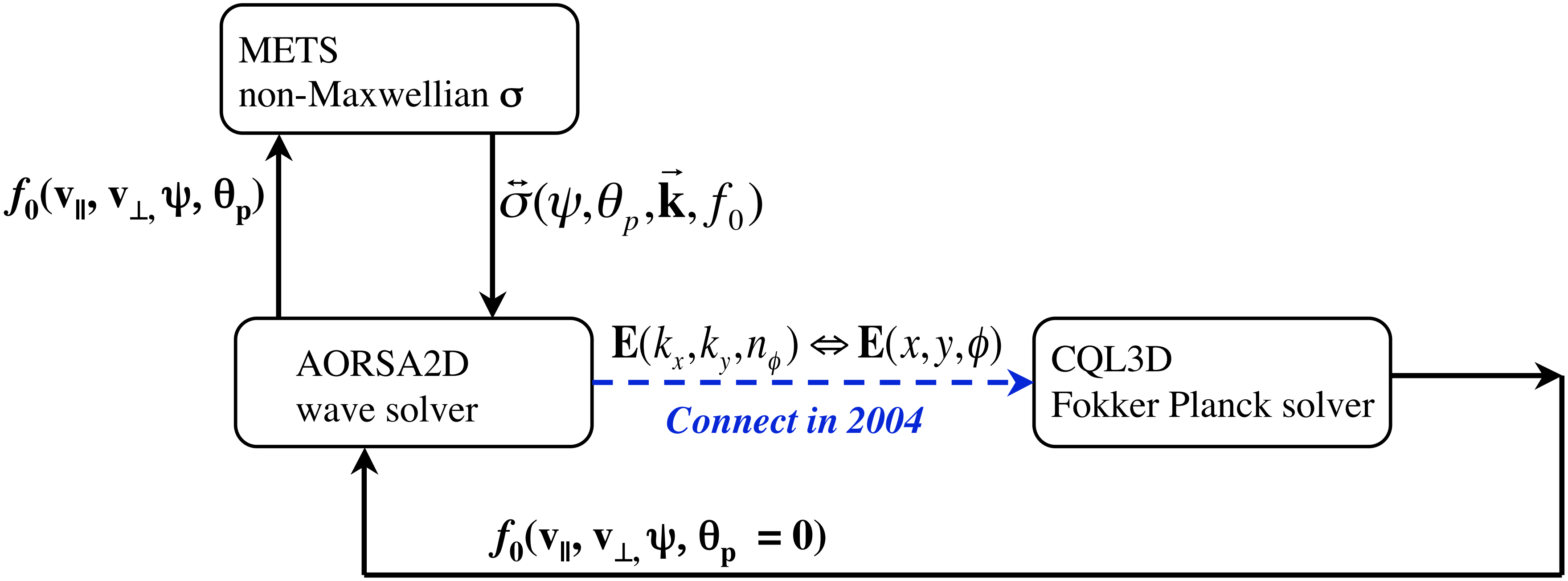
Electron absorption



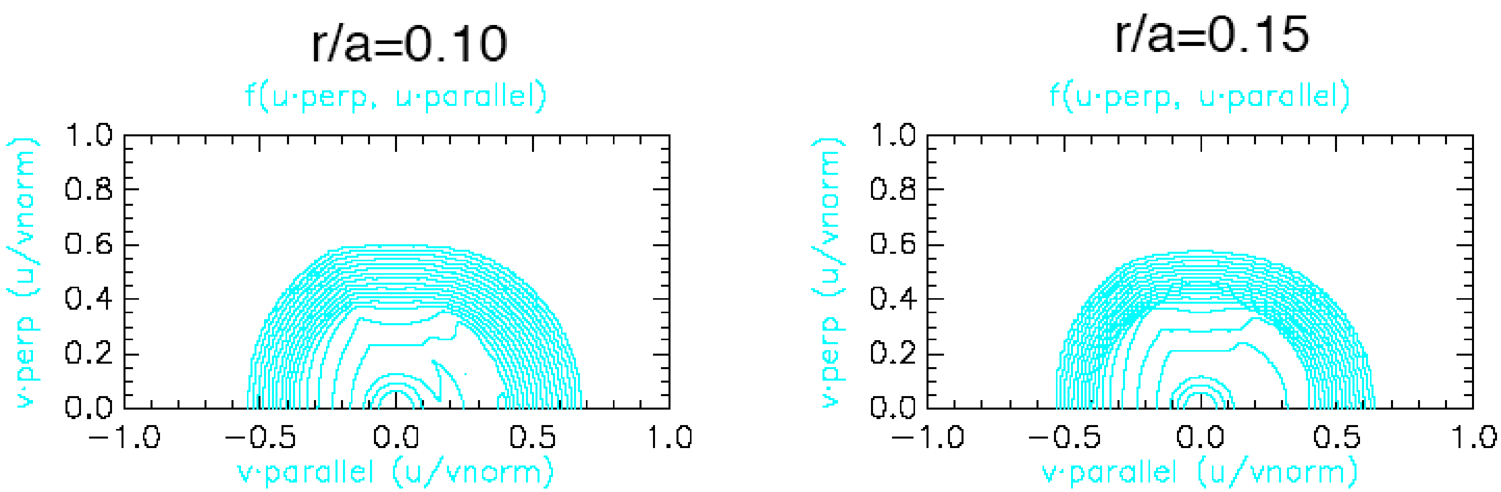
- **Without beam: 70 % (per pass)**
- **Isotropic beam: 24 %**
- **Anisotropic beam: 44%**

- **Isotropic slowing down and equivalent Maxwellian in agreement**
- **Wave absorption is strongly modified by inclusion of model anisotropic fast ion distributions**
- **Significantly less fast ion absorption predicted in the case of tangential injection**
  ⇒ implies less degradation of HHFW-CD efficiency

Non-Maxwellian conductivity has now been incorporated into AORSA codes, with numerical $f_0(v_{\parallel}, v_{\perp})$ from CQL3D code

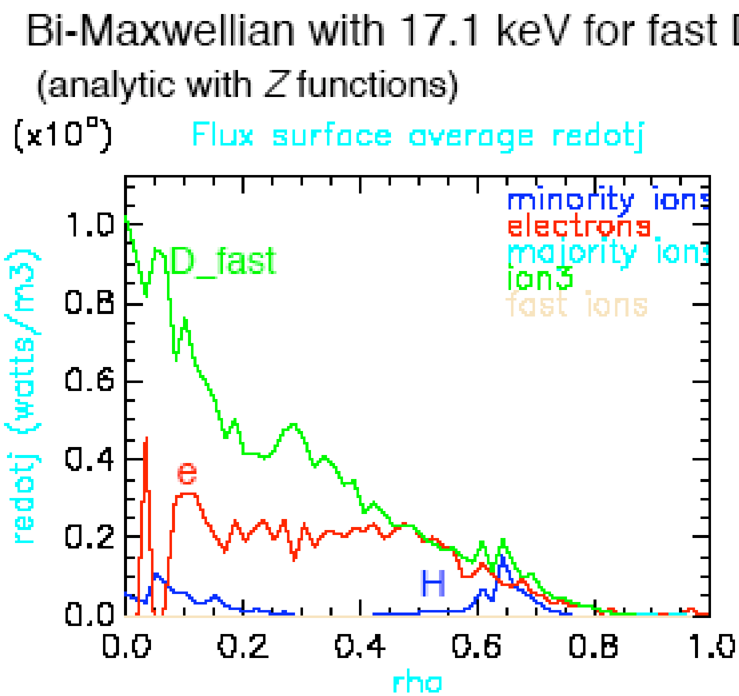


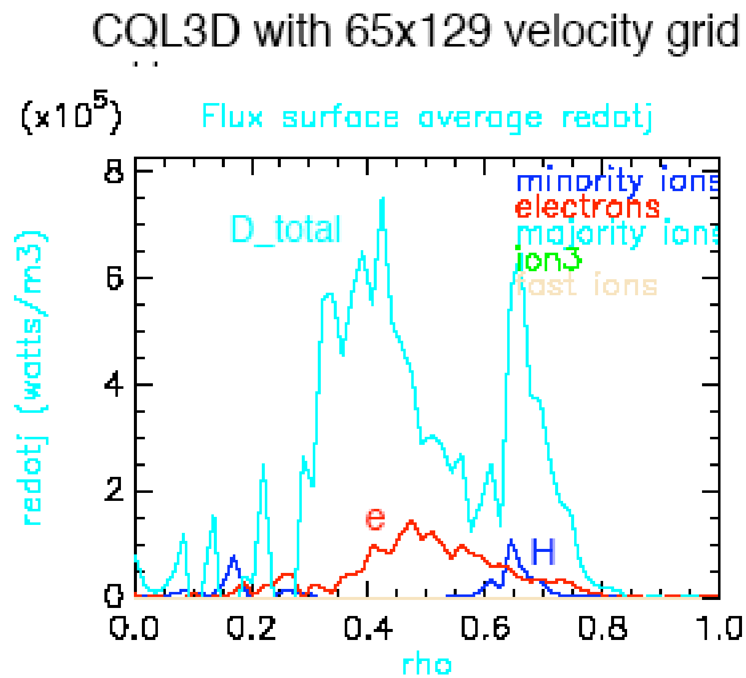
CQL3D distribution for NBI on NSTX (no RF)



We are beginning to get results from AORSA2D with numerical distribution functions

HHFW heating on NSTX with D beam injection:
Comparison of DQL3D 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**

CQL3D: Bounce-averaged Fokker-Planck Code

Solve for bounce-averaged distribution at torus equatorial plane ($\theta_P = 0$), $f_0(\rho, v_{||}, v_\perp, t)$

$$\frac{\partial(\lambda f)}{\partial t} = \frac{\partial}{\partial \mathbf{v}} \cdot \left[\Gamma_E + \Gamma_{RF} + \Gamma_{coll}\right] + R(f) + S_{NB} + S_{NB} + L$$

ρ = generalized radial coordinate labeling (non-circular) flux surface

λ = field line connection length

Γ_E = velocity space flux due to toroidal electric field (Ohmic)

Γ_{RF} = $\vec{\mathbf{D}}_{QL} \cdot \frac{\partial f}{\partial \mathbf{v}}$ = velocity space flux due to full, bounce average, RF Quasi-linear operator (all hamonics, Bessel functions, all wave modes)

Γ_{coll} = full, nonlinear, 2D, relativistic collisional operator

R(f) = Radial diffusion and pinch operator with v dependent coefficients

S_{NB} = Monte Carlo neutral beam source (NFREYA)

S_{KO} = Knock-on collisions (for electrons)

L(v) = velocity dependent prompt loss term

- **Implicit solve in ρ, $v_{||}$, $v_\perp$. Operator splitting in 3D cases.**
- **2D full wave RF fields are being imported in a "local spectral representation"**

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 macrosopic 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

$$P_{loc}(x) = \tfrac{1}{2} \operatorname{Re} J(x) \cdot E(x)$$

- 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

$$P(x) = \tfrac{1}{2} \operatorname{Re} \sum_{n,m} e^{i(k_n - k_m)x} W(k_n, k_m) E_n E_m^*$$

- In 2D this is 6 nested sums (8 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

Summary

- **There have been a number of other advances that I have not covered that might be of interest:**
  - **Rigorous 2D theory of RF induced fluid force for flow drive analysis**
  - **Improvement of threatment of parallel RF response – generalized Z function**
  - **Exploration of alternative field basis sets – splines, wavelets, Gabor transforms**
  - **Calculation of quasi-linear operator by direct integration of particle orbits in 2D wave fields**
- **We have begun to explore full-wave phenomena in 2D and 3D with much improved resolution and physics**
  - **Mode conversion in 2D**
  - **Fast wave heating in 3D**
  - **Effects of non-Maxwellian distribution**
- **To make feasible the integration of advanced RF models with other disciplines, such as transport or stability, or to carry out extensive studies within RF, careful attention to code speedup and optimation**
  - **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**

Roadmap for the next 3-year phase of SciDAC

- 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
  - fast particle effects on plasma rotation
  - providing source terms for neoclassical modeling e.g. NCLASS
  - flow drive interaction with turbulence and internal transport barriers
- Preparation for burning plasma experiment
  - Any burning plasma experiment, including ITER, will be a driven system ($Q \leq 10$) under most or all of it's operation
  - Validation and optimization of 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

Fusion Simulation Project (FSP) – The US is considering a major initiative in fusion simulation

- **"The purpose is to make a significant advance toward the ultimate objective of fusion simulation – to predict in detail the behavior of any discharge in a toroidal magnetic fusion device on all important time and space scales."**
- "The initiative should be planned as a 5-6 year program" – first phase of a ~15 year project
- "Rough estimates are that an integrated simulation initiative would require a total funding level of about $20 million per year, with funding for the plasma scientists provided by OFES and funding for the applied mathematicians, computer scientists, and computational resources provided by OASCR."
- **There are fundamental issues of fusion physics that have so far severely limited our ability to integrate the disparate physics models required for a comprehensive simulation. These include:**
  - **Extreme range of relevant time scales**
  - **Extreme range of relevant space scales**
  - **Extreme anisotropy of hot magnetized plasmas**
  - **Differing dimensionality of the relevant models**
  - **Non-linear coupling of phenomena**
- **In addition there are stringent requirements on the integration framework (or frameworks) for extensiblity, flexibility, and human and computational efficiency**

Realistically we do not now know how to construct a simulator that satisfies the ultimate requirements for physics and computational integration.

The approach is to begin the project with several (~ 4) Focused Integration Initiatives

- **Each initiative has 2 goals:**
  - **To develop computationally feasible solutions to one or more of the "fundamental" issues, such as multiple time scale**
  - **To develop an extensible computational framework for multi-physics simulation**
- **The traditional modeling disciplines that structure our understanding of fusion plasmas include:**
  - **plasma sources**
  - **turbulence**
  - **extended MHD**
  - **1.5D (one and one-half dimensional) transport**
  - **atomic physics**
  - **fusion materials**
- **Each focused initiative should cut across and integrate two (or a few) of these traditional disciplines, to provide physics integration both spatially and temporally**
- **Each initiative should address a compelling problem in fusion science physics that requires integrated simulation.**

Models of wave-plasma interaction will be an essential element all across the FSP

Examples of possible focused Integration Initiatives which cut across the usual fusion theory disciplines