Recent Results from the SciDAC Partnership for Simulation of Fusion Relevant RF Actuators

P. T. Bonoli and D. L. Green on behalf of the RF-SciDAC Team

2019 Scientific Discovery through Advanced Computing (SciDAC-4) Principal Investigator Meeting

July 16-18, 2019
Rockville, MD

RF-SciDAC : Center for Simulation of Fusion Relevant RF Actuators
http://rfscidac4.org

Partnership is a collaboration of FES and ASCR participants from DoE laboratories, universities, and private companies

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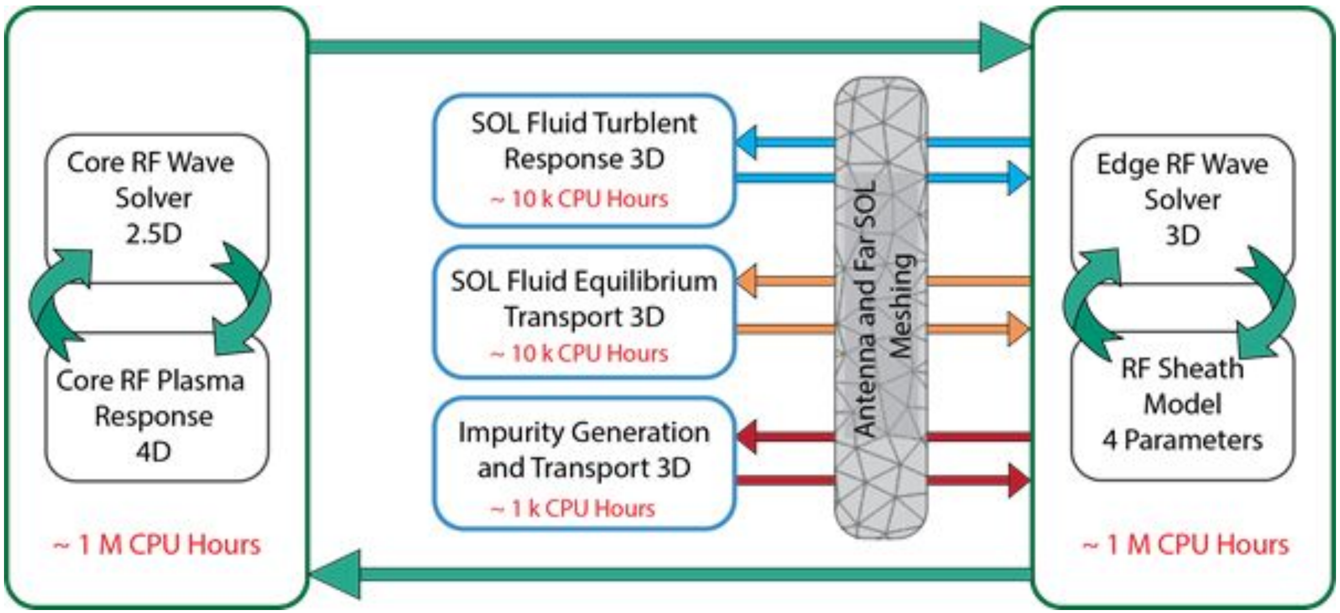
  - **ASCR:** T. Kolev, M. Stowell, D. Copeland, V. Dobrev, A. Friedman, S. Petrides
- **Tech-X**
  - D. N. Smithe, T. G. Jenkins
- **CompX**
  - R. W. Harvey, Yu. Petrov
- **Lodestar Research**
  - J.R. Myra
- **Rensselaer Polytechnic Institute**
  - **ASCR:** M. Shephard, M. Hakimi, U. Riaz
- **University of Illinois - Urbana Champaign,**
  - D. Curreli

RF-SciDAC

Scientific objective: Develop simulation capability to predict the self-consistent interaction of RF power with the core plasma, scrape off layer and wall



- Include the effects of ponderomotive density modification and fluid turbulence and transport.
- Predict high-Z impurity sputtering and transport induced by large RF-induced sheath potentials, and associated localized thermal loads, to guide development of impurity mitigation strategies for ITER.

RF-SciDAC

Project is organized into four main thrust areas led by FES and ASCR personnel in order to accomplish our scientific objectives

- **Thrust 1: RF WDM Components (for AToM & TRANSP) and Thrust Common Efforts**
    - N. Bertelli (FES) / E. D'Azevedo (ASCR)

- **Thrust 2: RF + Turbulence**
    - A. Dimits (FES) / J. Myra (FES)

- **Thrust 3: RF + Equilibrium Transport**
    - J. Lore (FES) / M. Stowell (ASCR)

- **Thrust 4: RF + Impurity Generation**
    - J. Wright (FES) / D. Curreli (FES)

RF-SciDAC

I. High fidelity RF wave solver for the fusion edge

- MFEM based mini app wave solver (Stix Mini-App)
  - RF sheath boundary conditions (BCs)
- Pre-conditioner (PC) studies
  - Physics based - WKB
  - Algebraic
  - Domain decomposition
  - Reduced precision
- MFEM based full fidelity wave solver (Petra-M)
  - Meshing
    - CAD to useful computational mesh
    - High geometric fidelity
    - Coupling to MFEM
    - Adaptivity

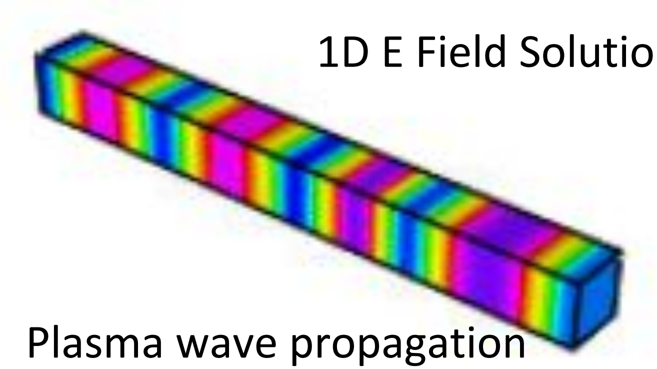
Stix Mini-App : Overview

- MFEM test bed for developing advanced methods.
- Plasma wave equation solver in 1D and 2D (work in progress)

$$\frac{1}{\mu_0}\nabla \times \nabla \times \vec{E} - \omega^2 \epsilon_0 \vec{E} + i\omega\vec{\sigma}\vec{E} = -i\omega \vec{J_{ext}}$$

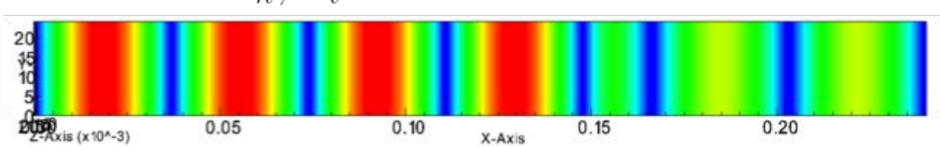
- Current Boundary Conditions supported:
  - Conducting (1D, 2D)
  - Absorbing (1D, 2D)
  - Linear finite sheath (1D)

1D E Field Solution



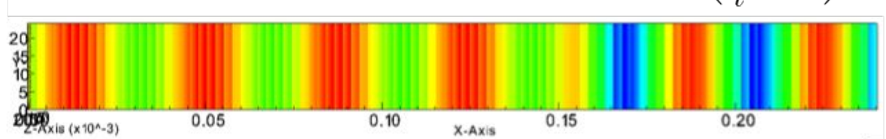
Plasma wave propagation

PEC BCs $E_n, E_t = 0$



Imaginary E Field Components w/ Conducting Wall

Linear RF sheath BC $E_t = \nabla_t \left(\frac{\omega}{i} D_n z\right)$



Imaginary E Field Components w/ Sheath BC

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Stix Mini-App : Current and Future Work

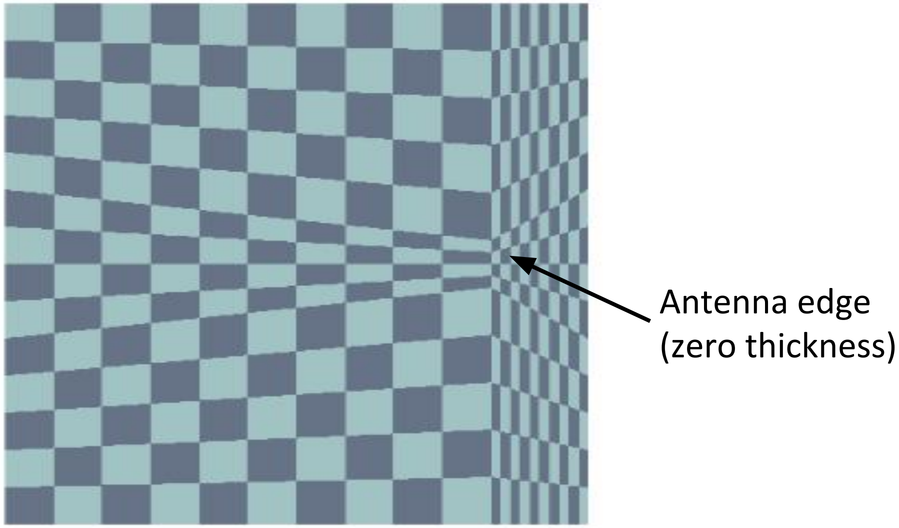
- Nonlinear finite sheath width BC:

$$E_t = \nabla_t \left(\frac{\omega}{i} D_n z \right) \quad \text{where} \quad \frac{1}{z} = \frac{\langle J V_1 \rangle}{\langle V_1^2 \rangle} - \frac{i\omega \langle J \dot{V}_1 \rangle}{\langle \dot{V}_1^2 \rangle}$$

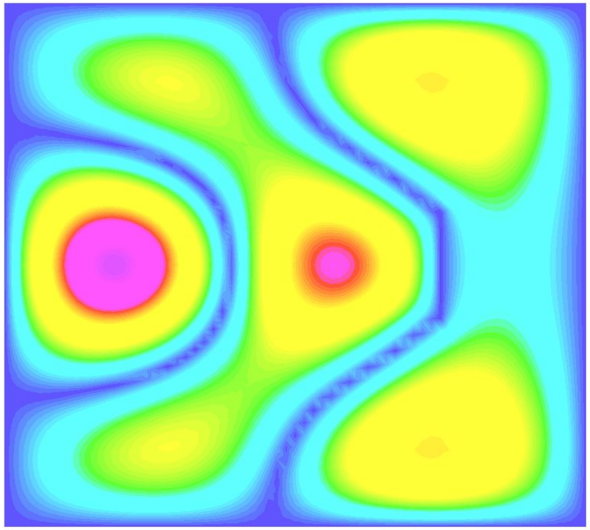
[J. Myra, et al., Phys. Plasmas 22, 062507 (2015)]

- Non-uniform density in propagation direction.
- Investigate preconditioners.
- Investigate mesh adaptivity criteria.

Example mesh



E field solution of mesh

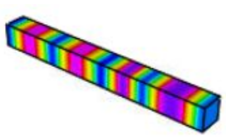


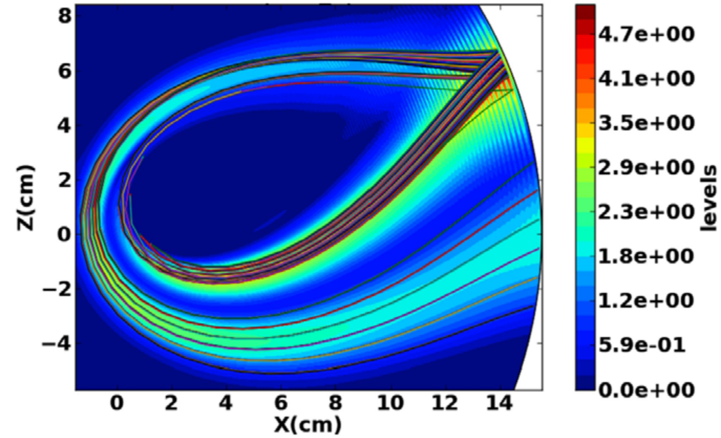
Preconditioners I

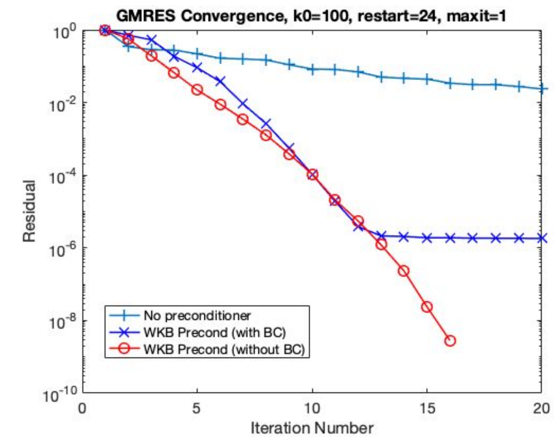
- High geometric fidelity (antenna structure), multiple wave scales (slow and fast), and 3D mean O(10^8) DOF.
  - We need a preconditioner for

$$\nabla \times (\mu^{-1} \nabla \times \vec{E}) - \omega^2 \epsilon \vec{E}$$

  - Difficulties include large null space of curl curl operator and anisotropy in dielectric tensor.
- Physics based - WKB
  - Use ray-tracing to approximate solution.
  - Shows promise in 1D.
- Algebraic
  - Approximate dielectric.



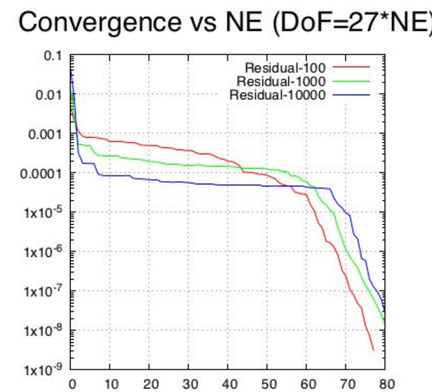




$$\nabla \times (\mu^{-1} \nabla \times \vec{E}) + \omega^2 \alpha \vec{E}$$

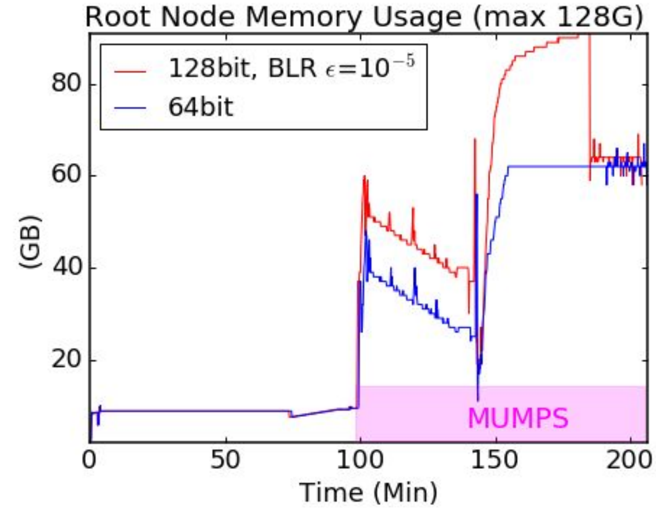
$$\alpha \equiv \begin{pmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & |P| \end{pmatrix}$$

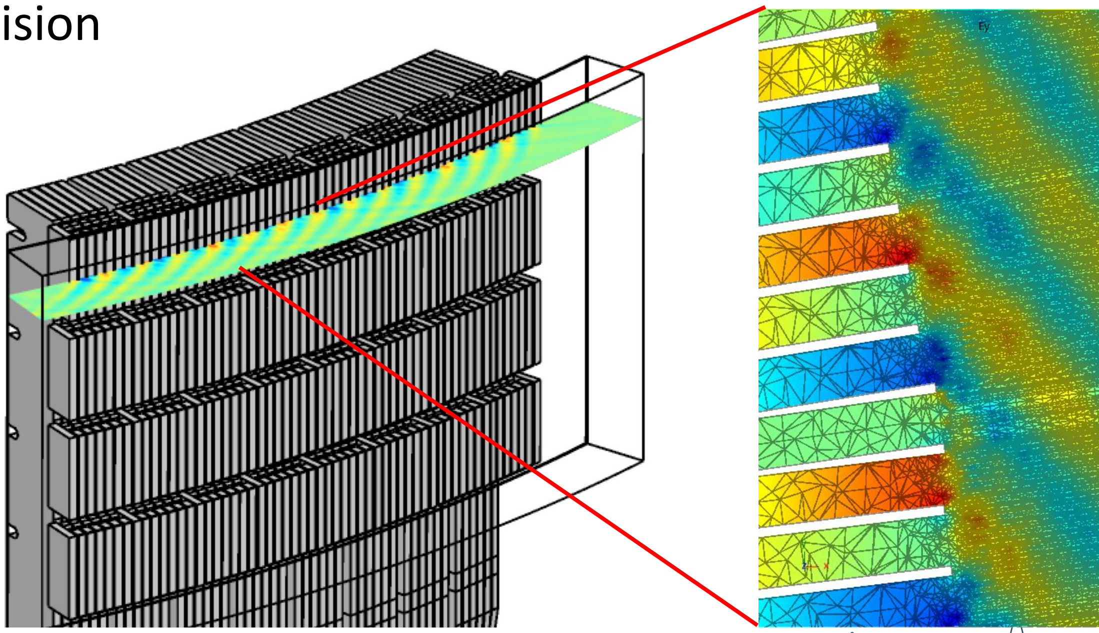
$$A \equiv \frac{1}{2}(|S + D| + |S - D|)$$



Preconditioners II

- Direct solve of smaller system as PC (Tested in Petra-M)
  - Low rank approximations
    - BLR (Block Low Rank) -red
  - Lowering floating point precision
    - Single precision - blue
  - 15-20 GMRES iterations
  - Enabled resolving LH wave scattering in 3D for DIII-D high field side lower hybrid launcher.





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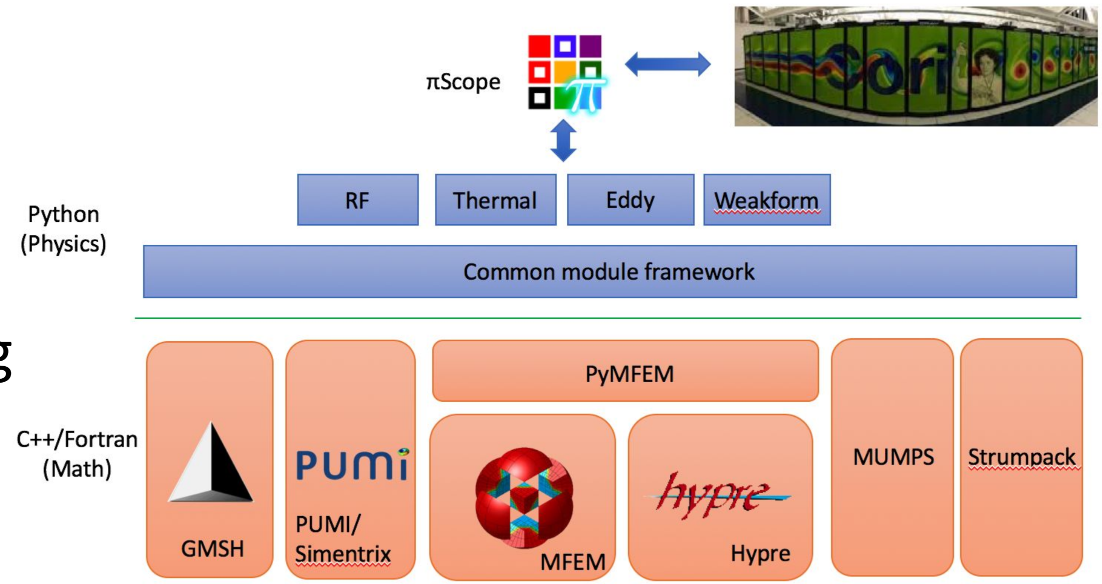
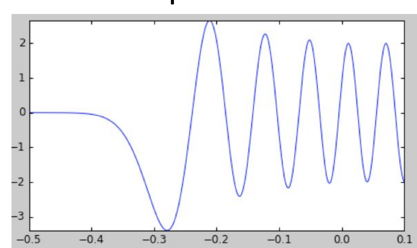
Petra-M : Physics Equation Translator for MFEM

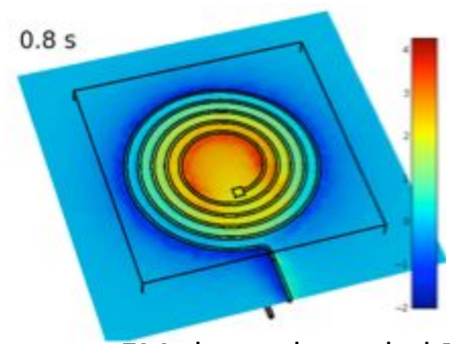
- FEM analysis platform
- Front-end interface to open source software
- Integrated FEM modeling from geometry to FEM assembly and solve.
- Deployment tool for our advanced physics model
  - Started as RF modeling tool and being applied in many RF problems in fusion experiments
  - Use case is even expanding outside RF waves.



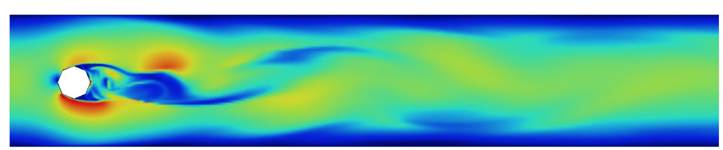
Petra-M examples



1D RF wave



EM-thermal coupled PDE



Navier-Stokes

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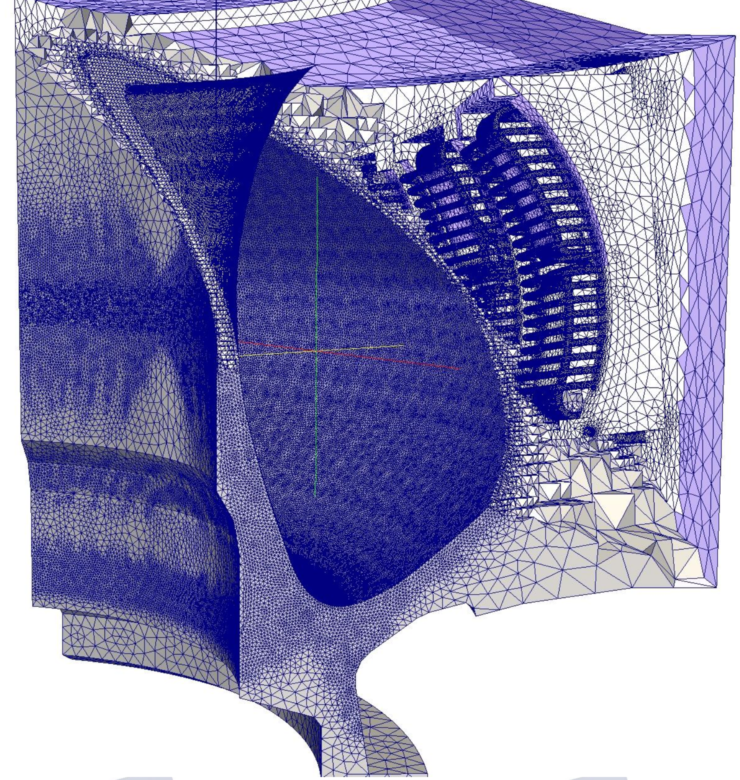
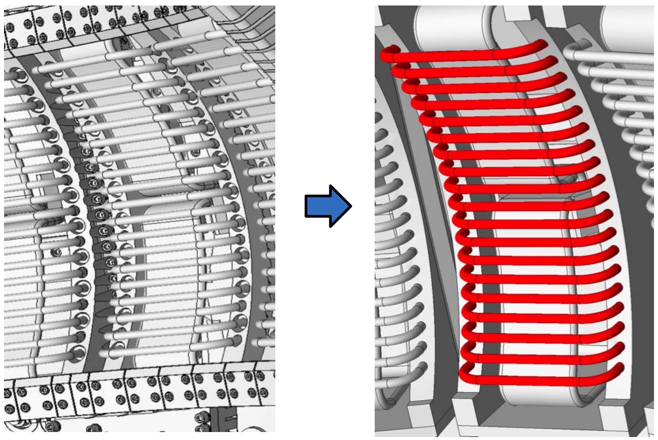
Meshing for the wave solver

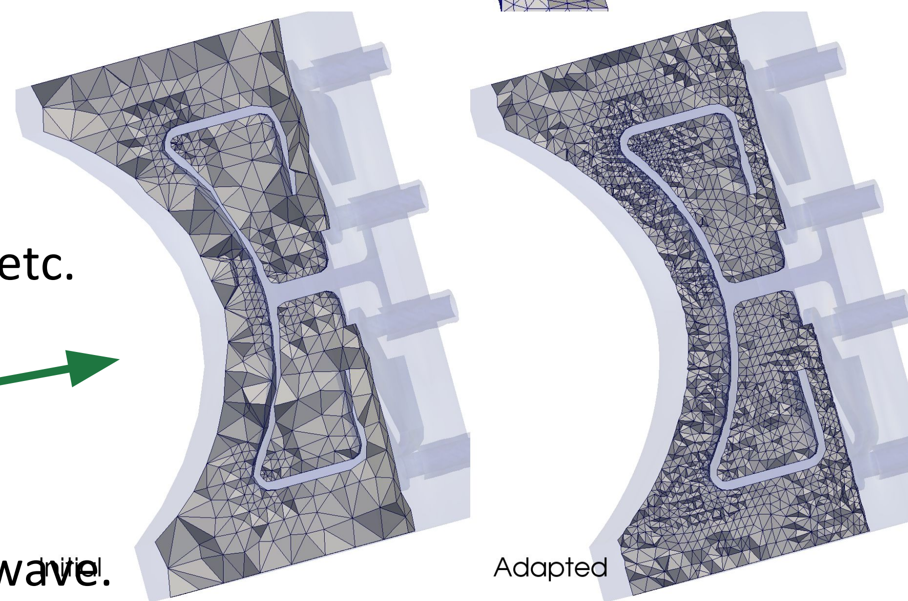


- CAD to useful computational mesh
  - Defeaturing



Defeaturing

- High geometric fidelity
  - Capture antenna / faraday screen etc.
- Coupling to MFEM
- Adaptivity
  - Next steps will look at slow + fast wave.



II. Equilibrium & Turbulent far-SOL Transport

- Braginskii mini-app
  - Evolve the background plasma in and around the RF hardware.
  - MFEM based far-SOL fluid transport solver.
  - Anisotropy to be handled via combination of high order elements and graded meshing from field aligned to geometry conforming.
- Meshing (field aligned / geometry conforming)
- SOLT-3D (BOUT++)
  - Ponderomotive Coupling to VSIM (Vorpal).
  - RF Sheath Potential Coupling.
- RF scattering from turbulence

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Braginskii Mini-App : New fluid plasma transport solver based on MFEM

- Physics Model
  - Classical parallel transport, cross-field drifts, ad-hoc perp diffusion.
  - Two-fluid model (single ion species and electrons).
  - Diffusion model for a single species of neutral atoms.
  - Currently neglecting drifts, recombination, ohmic heating, solves coupled equations for density, parallel momentum, electron and ion energy, (potential equation - from vorticity - coming soon).
- Computational Model based on MFEM
  - Coupled system of non-linear partial differential equations.
  - Discontinuous Galerkin Finite Elements of arbitrary order.
  - Time integration using high-order SDIRK methods.
  - Time step set using Proportional-Integral-Derivative (PID) Controller.
  - Adaptive mesh refinement based on weighted error estimates.

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Testing high order basis functions for anisotropy

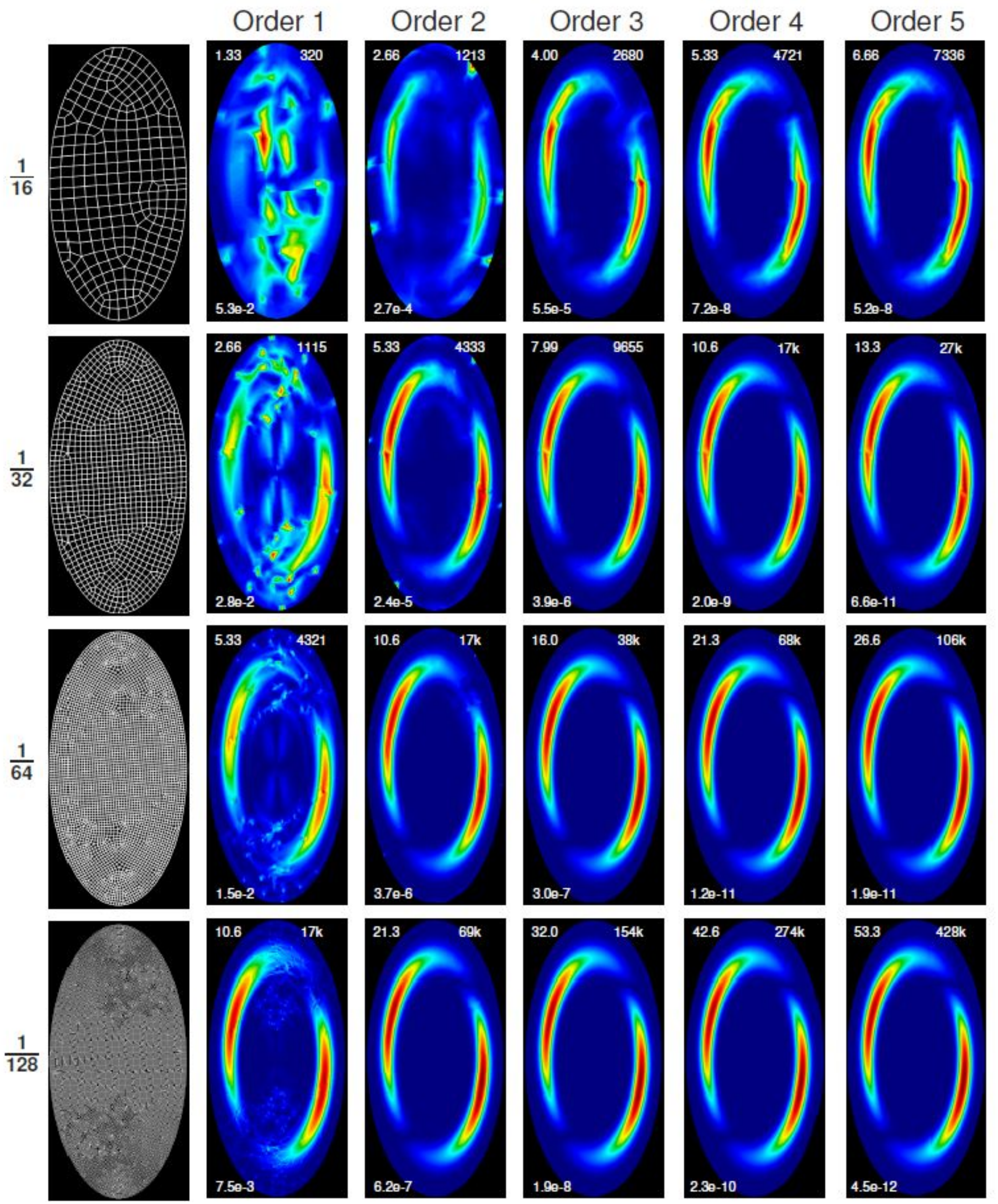
- Plasma transport is highly anisotropic.
- High order basis functions tested in using MFEM.

$$c_p \frac{\partial T}{\partial t} - \nabla \cdot [\chi \nabla T] = Q$$

Where χ is an anisotropic tensor given by: $\chi = \chi_\perp \left(I - \hat{n}\hat{n}^T\right) + \chi_\parallel \hat{n}\hat{n}^T$ with $\chi_\parallel \gg \chi_\perp$

- $\chi_\parallel / \chi_\perp = 10^3, \ldots, 10^9$
- Mesh densities $h = \frac{1}{16}, \ldots, \frac{1}{128}$
- Basis function orders $p = 1, \ldots, 5$
- Need > 16 interpolation points across features of interest

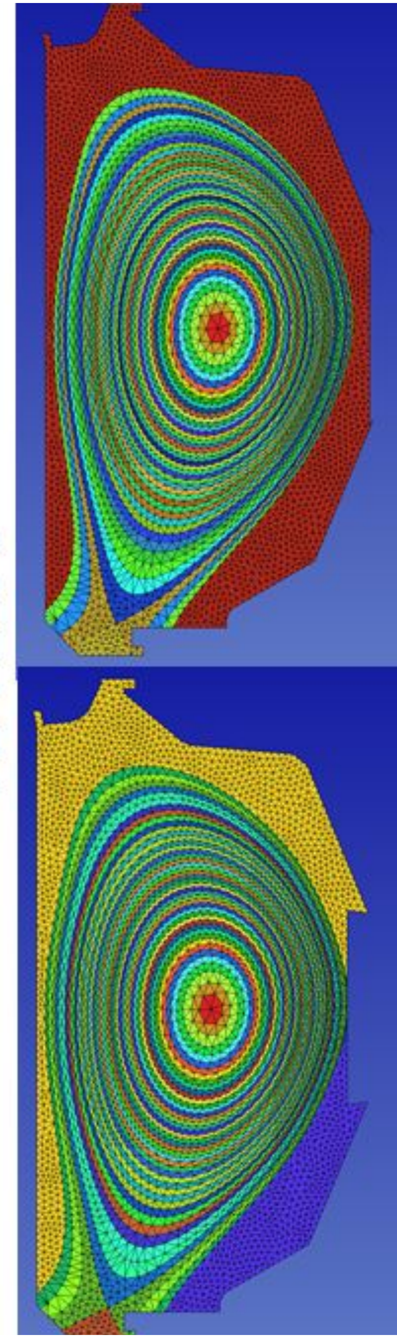
Parallel Diffusion Results for $\chi_\parallel / \chi_\perp = 10^9$

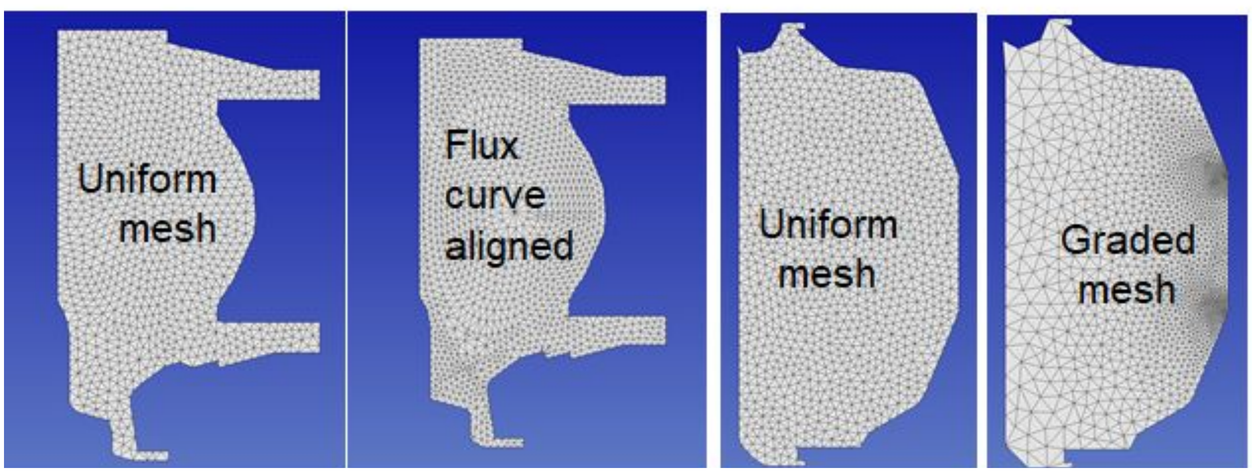


Geometry and Unstructured Meshing

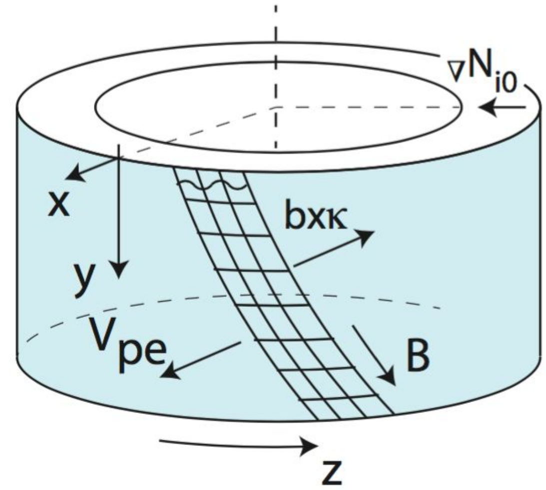
- On going meshing activities
  - **Goal is to grade from field aligned to geometry conforming to aid with the anisotropy issues.**
  - Performing initial tests on realistic geometries.
  - Comparing alternative mesh configurations
    - Unstructured meshes with general mesh gradations.
    - Unstructured meshes with alignment to flux surfaces.
    - Meshing modified geometries.

Flux surface aligned mesh
Top – original geometry
Bottom – modified Geometry

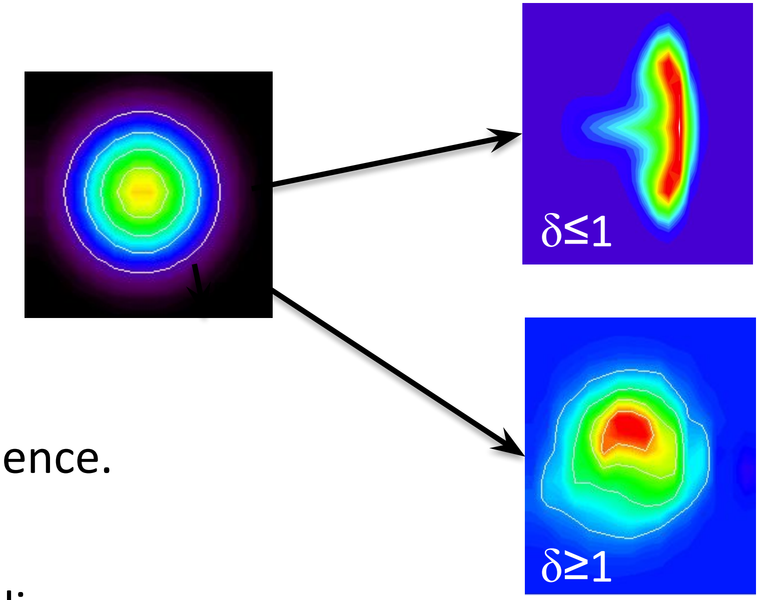




RF interaction with fluid turbulence



- SOLT3D (BOUT++ model) provides a simple & verified model for SOL fluid turbulence.
  - Implements the drift-reduced-ballooning fluid Equations, including curvature drive, and divertor-plate sheath BC’s in simplified geometry.
- SOLT3D blob simulations agree with previous published results
  - Small blobs δ<<1 (KH mushroom breakup)
  - Large blobs δ>>1 (interchange breakup)



- Can now be used for
  - RF scattering from turbulence.
  - Add RF source terms.
  - Ultimately two-way coupling.

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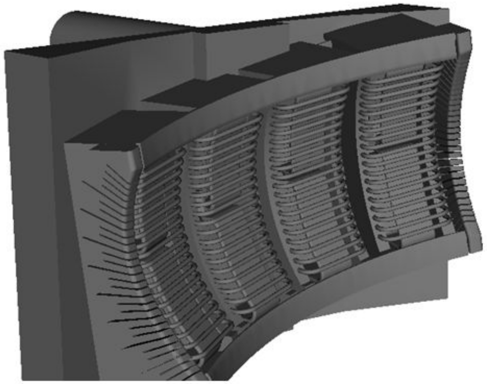
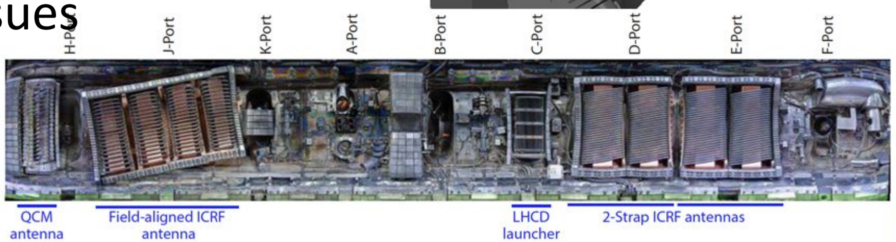
Coupling of wave solver (VSIM) and turbulent transport (SOLT3D)

- Ponderomotive Force
  - |Amplitude|^2, steady-state "pressure" from the RF's |E|^2, |B|^2, and |JRF|^2 energy, as it propagates through the steady-state plasma.
    - Fast wave, E ~ 5.0×10^4 V/m --> Like 0.1eV
    - Slow wave, E ~ 1.5×10^5 V/m --> Like 1eV
  - If slow waves are present, will they cause density rarefaction in front of antenna, thus perpetuating the low density that favors the slow wave.
  - Can be extracted via lo-pass filter of VSIM wave field output
  - First, we are testing SOLT3D with analytical model terms that mimic output expected from Vsim
  - Direct coupling will follow once issues explored with model

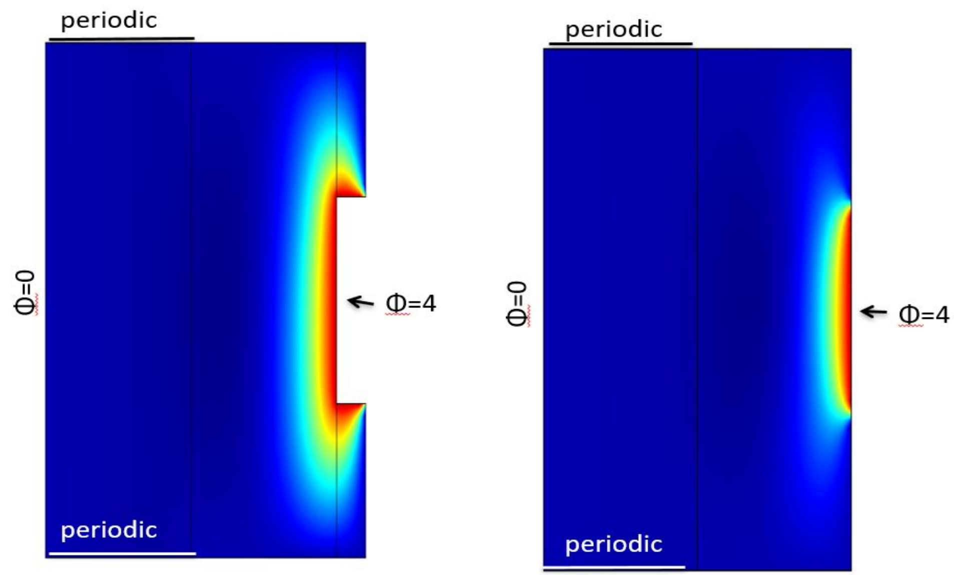




$$\mathbf{F}_s \equiv \rho_{s1}\mathbf{E}_1 + \mathbf{J}_{s1}\times\mathbf{B}_1 - ({}^m/_q)_s \nabla\cdot\left[\frac{\rho_{s0}^2 \mathbf{V}_{s1}\mathbf{V}_{s1}}{\rho_{s0}+\rho_{s1}} \right]$$

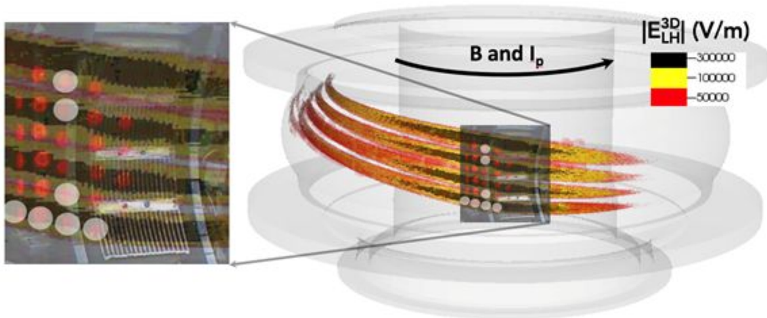
Progress has been made on implementation of RF-sheath boundary conditions in BOUT++ (SOLT3D)

- Want to study effects of boundary conditions resulting from RF launching structures on turbulent solutions e.g., from SOLT3D.
- Presently available BOUT++ mesh classes do not allow for impinging structures.
- Spatially dependent boundary conditions on an outer flux surface may be adequate.
- Use steady solutions of the SOLT3D model implemented in a FEM package (presently COMSOL) to determine boundary conditions on a flux surface, given those at the material surfaces.

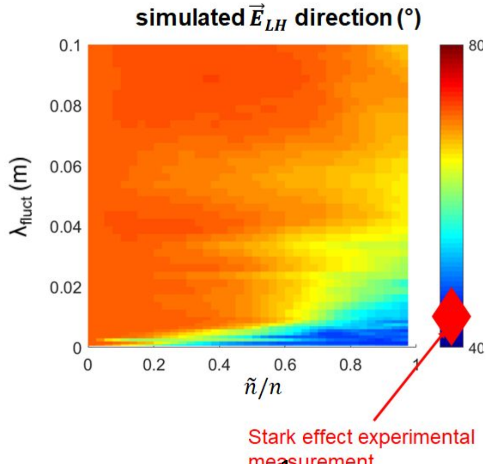


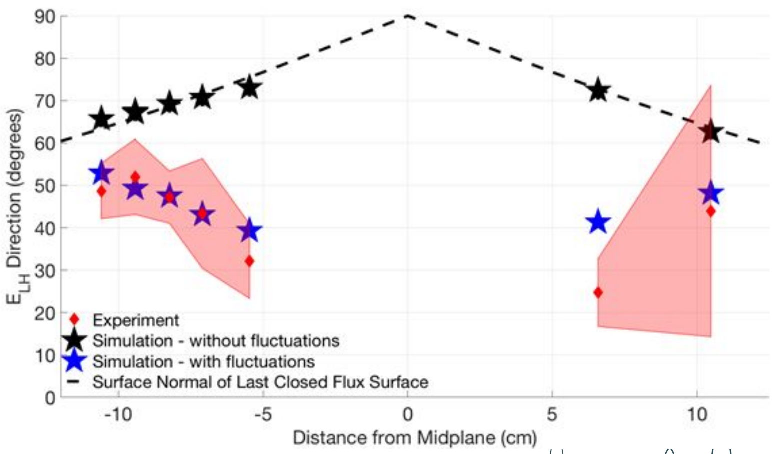
RF simulations suggest scattering from turbulent fluctuations may explain experimental observations

- New dynamic Stark effect spectroscopy measurement technique developed to measure magnitude and direction of $\bar{E}_{LH}$ on Alcator C-Mod[1,2]



- Without synthetic fluctuations, measurement and RF simulation agree for magnitude, disagree for direction of $\bar{E}_{LH}$
- With synthetic fluctuations, there could be much better agreement between measurement and RF simulation for direction of $\bar{E}_{LH}$





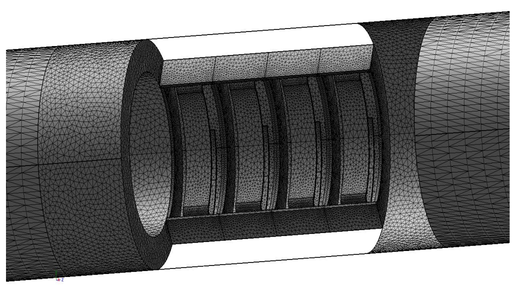
[1]Martin et. al, IAEA2018, [2]Martin et. al, NF2019

III. 3D FEM RF simulation model deployment and validation using high fidelity wave solver (Petra-M)

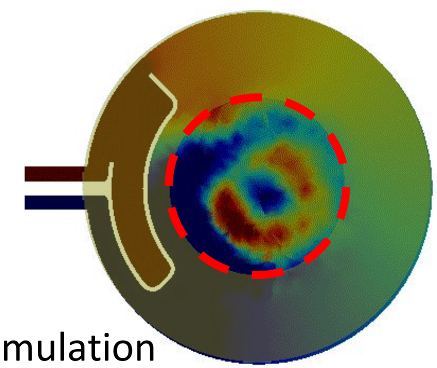
- LAPD RF Campaign.
- LAPD HHFW antenna simulations.
- Full torus HHFW simulation for NSTX.
- ICRF antenna modeling for JET ITER-like antenna.

LAPD : RF campaign studies RF wave physics relevant to fusion

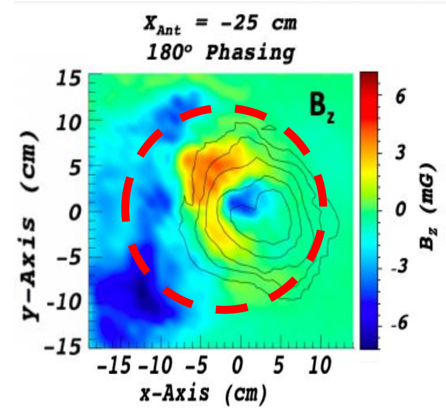
- High level physics goals include:
  - Validate linear, 3D RF simulation.
  - Collect benchmark dataset to validate non-linear RF physics theory/models (RF sheaths, ponderomotive forces, turbulence etc.)
  - RF campaign expecting 4 run weeks / year for 2019 - 2021.
- Joint effort by GA, MIT, ORNL, PPPL, RMA, TAE.
- **RF wave excitation by 4 strap HHFW antenna was modelled and compared well with experiment qualitatively:**



Simulation

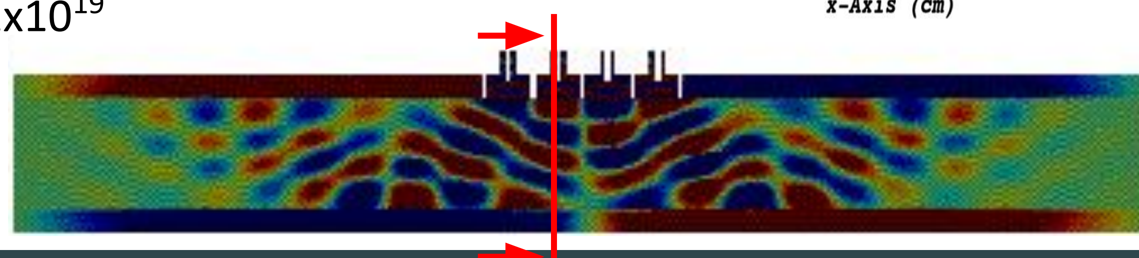


Measurement



f = 1 MHz, $n_{e\_antenna} \approx 10^{18}$ m^{-3}, $n_{e0} \approx 2\times10^{19}$ m^{-3}

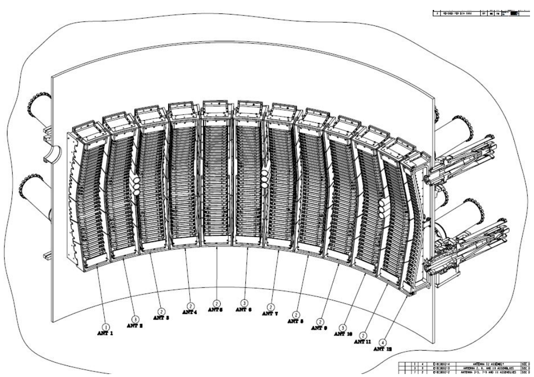
The B and E field are measured by scanning probes in front of antenna

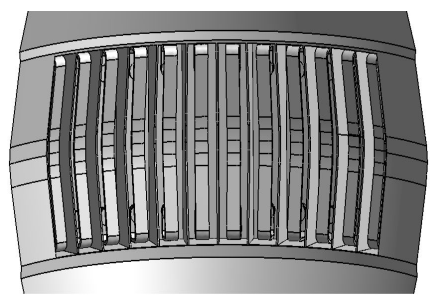


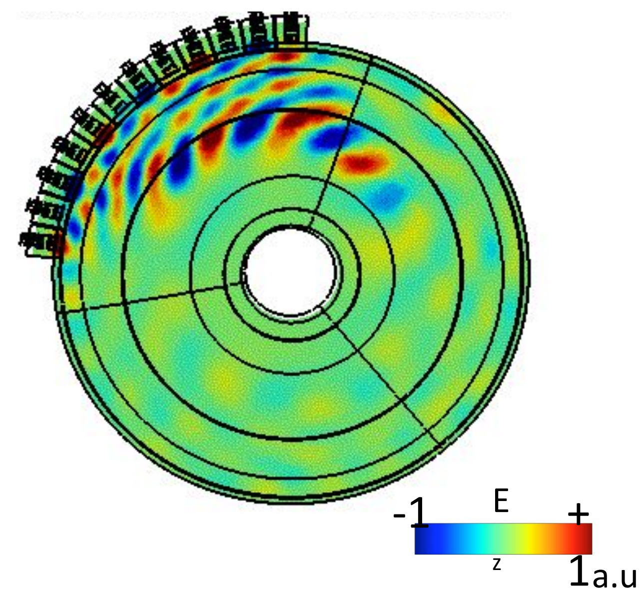
NSTX : First full 3D torus simulation including realistic antenna geometry

- Wave frequency = 30 MHz, Toroidal mode number = 12 ($|k_\varphi| = 8m^{-1}$)
- Analytical density profile with exponential decay in the SOL plasma
- Vacuum in the antenna box and anisotropic cold plasma in the torus with collisions

Can now handle the entire NSTX-U size tokamak plasma + complicated antenna structure together





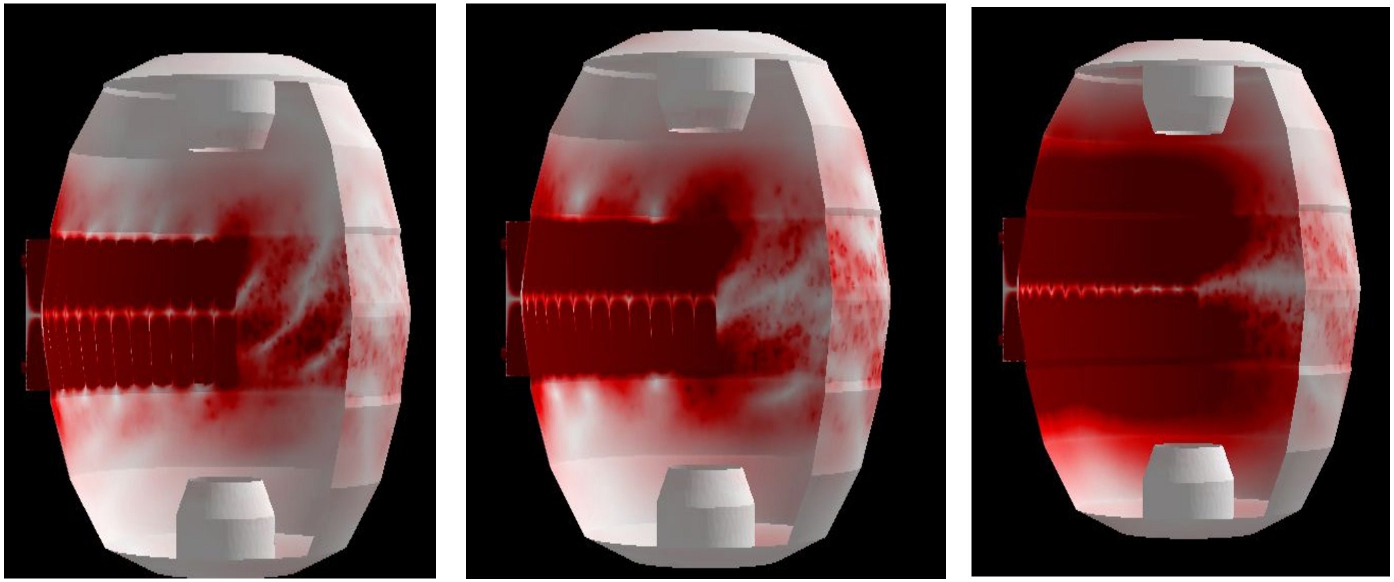


Physical + Magnetic geometries are generated from

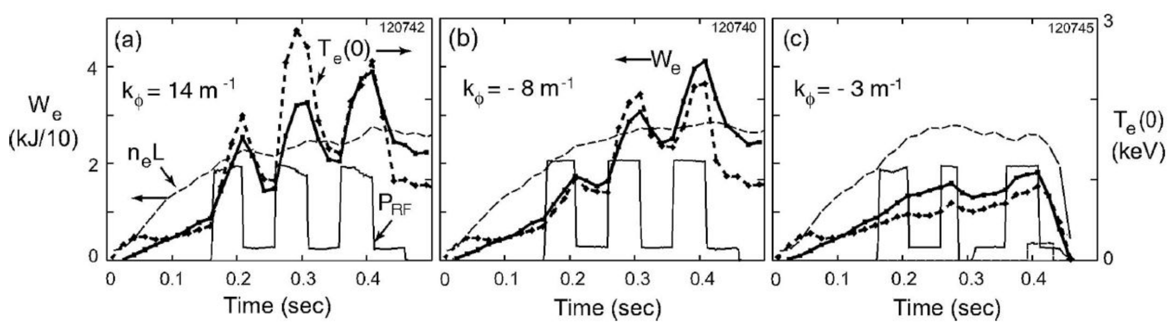
- Antenna engineering drawings
- Vacuum vessel
- Magnetic field configuration EFIT

NSTX : RF electric field on the wall surface is strong even far away from the antenna, in particular for lower phasing

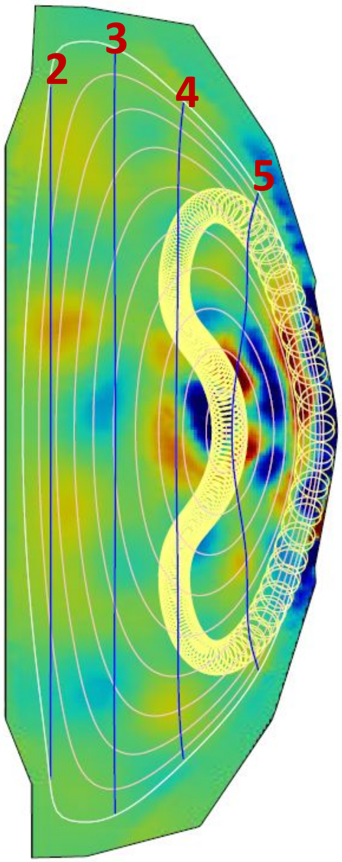
150° 90° 30°



- E field on the surface is stronger for lower antenna phasing
  - Consistent with poorer RF heating performance for low k_φ (Hosea PoP 2008)

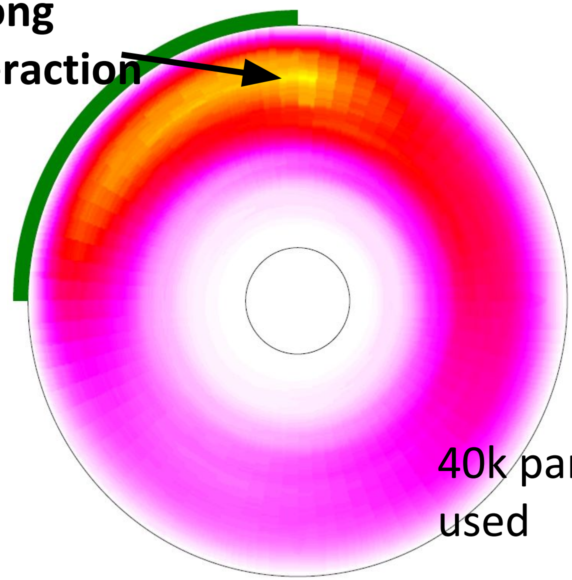


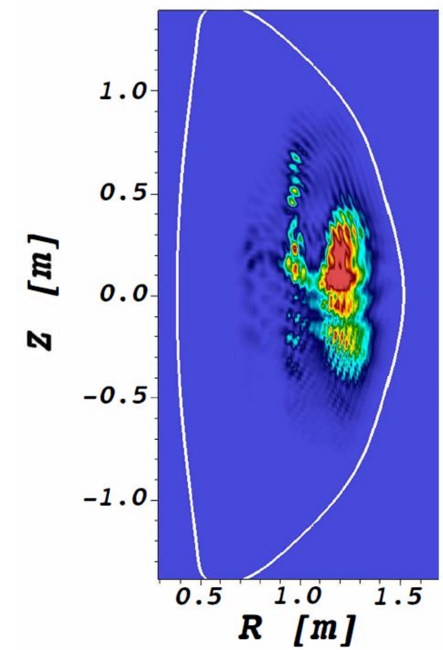
3D RF field from Petra-M combined with SPIRAL particle following code [1] to study the interaction of FW with fast ions in NSTX



$\mathcal{E}$ = 80 keV
$v_{||0}$=0 m/s
R_0 = 0.95 m
Z_0 = 0.6 m
(n=5 D resonance)

Assuming a Maxwellian in SPIRAL code with $T_{FI} \approx$ 25 KeV





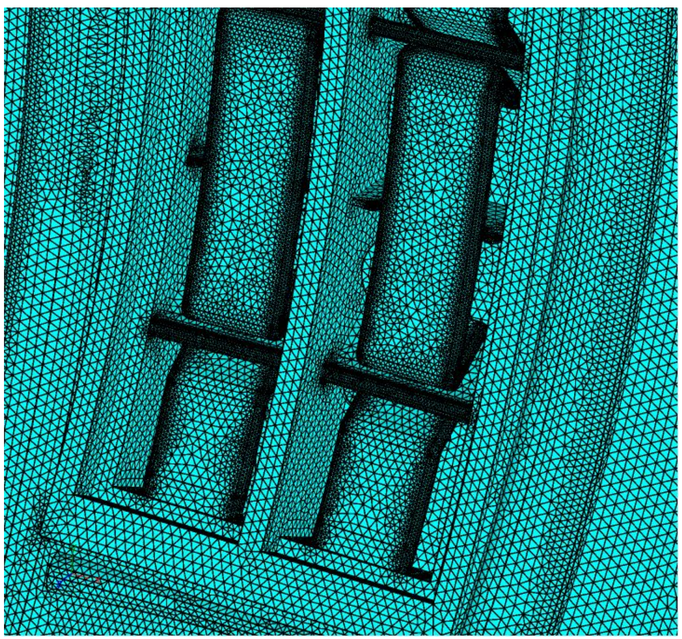
Strong interaction close to 5th harmonic D resonance appears similar to AORSA simulation

Fast ion power deposition predicted in AORSA assumes single n_φ and Maxwellian distribution function

[1] G. J. Kramer et al, PPCF **55** (2013) 025013

JET ILA : Collaboration to better understand RF-Wall interaction on JET ITER-like antenna has started

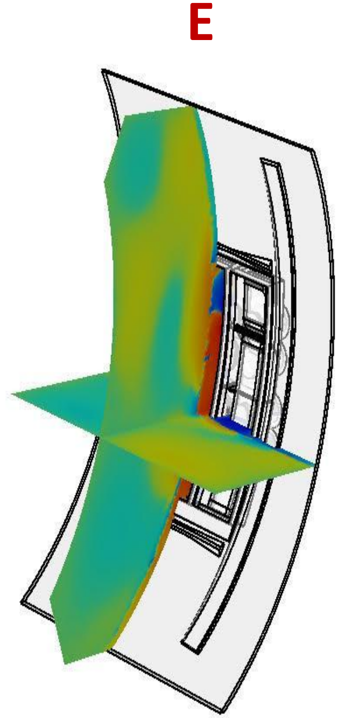
- Large complicated antenna module
  - 2 Toroidal/4 Poloidal antenna structures.
  - 6 Separators.
  - 8 feeding port structure.



Initial simulation demonstrated 3D antenna model with plasma load

- f = 42 MHz
- B = 2.85 T
- $n_{e\_antenna} \approx 2 \times 10^{18}\ m^{-3}$ [1]
- Antenna phasing = 0-pi
- Cold plasma
- Radiative load using collisions

[1] A. Křivská, et al, Nucl. Mat. and Energy **19** (2019) 324



- 3D Solid model was generated from the surface geometry data.
- **Next steps are to employ post processing sheath calculation and compare with impurity production diagnostic.**

IV. RF Sheaths and Sputtering

- Sub-grid RF sheath model - NoFlu
- Benchmarking kinetic vs fluid sheath models
  - NoFlu (fluid)
  - hPIC (Maxwell-Boltzmann electrons + kinetic ions)
  - Vorpal (kinetic electrons and ions)
- 1D RF sputtering model

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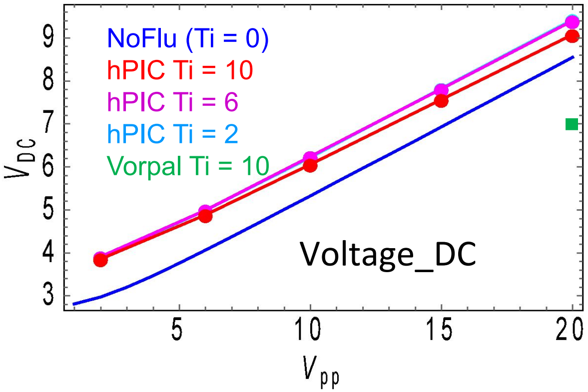
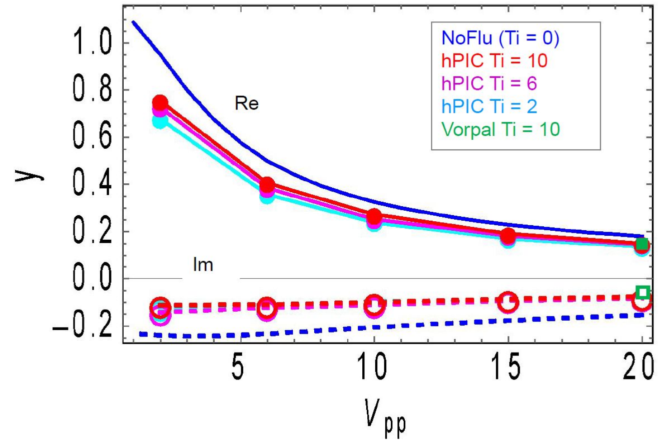
Parameterization of the sub-grid RF sheath model - NoFlu

- ICRF sheaths are associated with impurity production, etc.
- RF sheath adds nonlinearity to full-wave solvers.
  - Sheath controlled by the local RF wave fields.
  - RF wave fields are affected by the sheath.
- To avoid resolving the time and spatial scales of the RF sheath, a fluid model sub-grid BC (NoFlu) is under development.
  - Post processing (linear).
  - Incorporated into Stix mini-app (linear).
  - Incorporated into Stix mini-app (non-linear).
- The fluid sheath model is being validated with kinetic models (hPIC and Vorpal).
  - Finite ion temperature.
  - Spatial distribution of sources.
  - Non-Maxwell-Boltzmann electrons.

Sheath model benchmarking



Admittance



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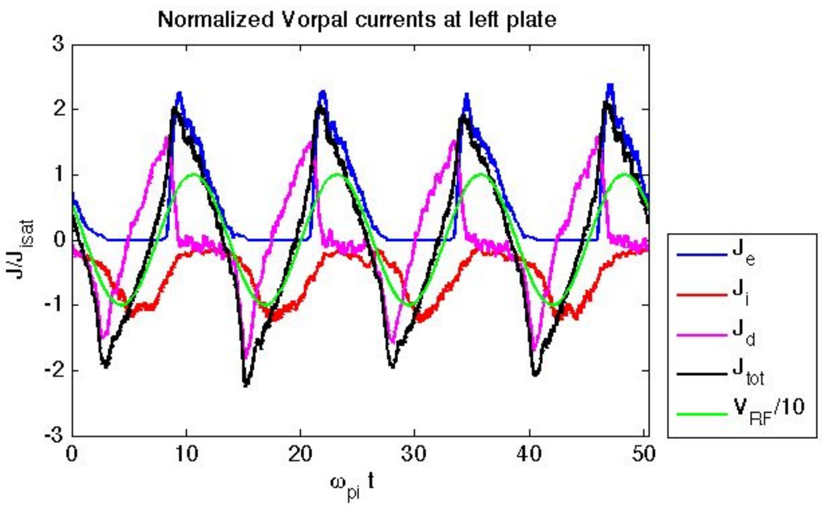
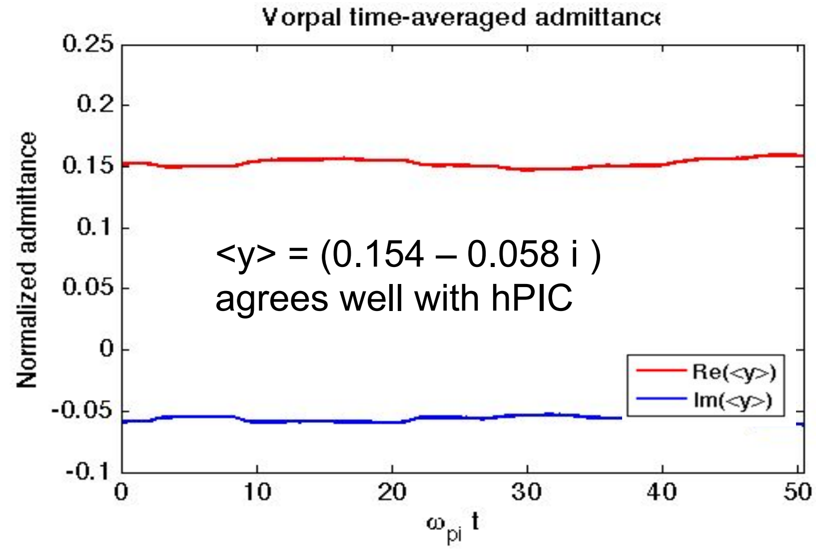
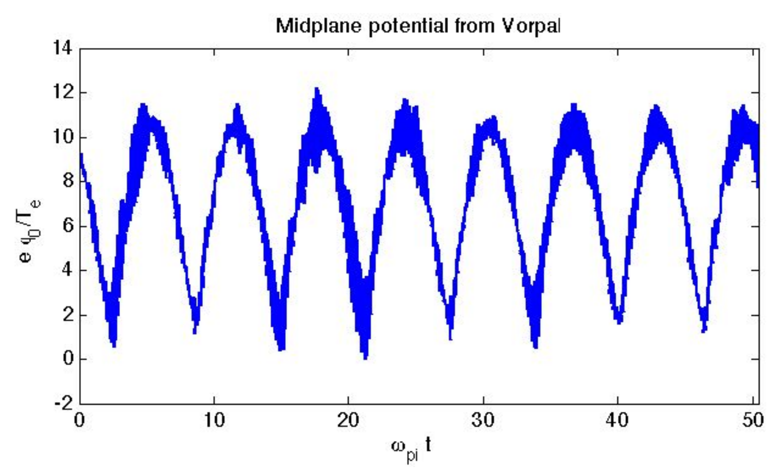
Vorpal modeling with kinetic electrons





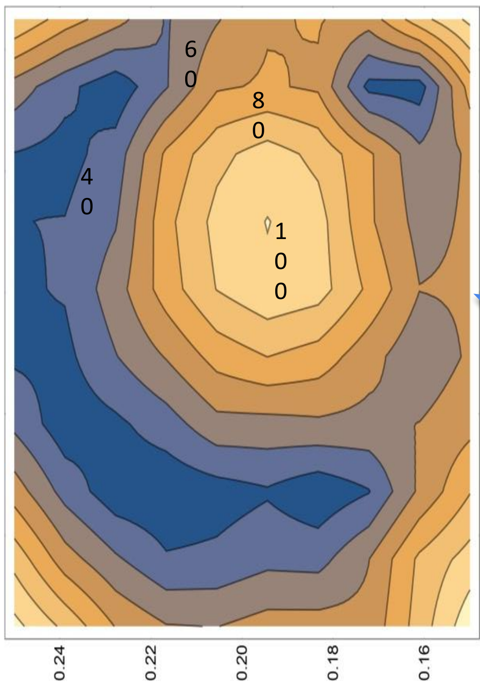
- Vorpal model for the sheath
  - Kinetic electrons and ions.
  - Increased computational resources.
  - 1x-3v.
- Current profiles qualitatively similar to hPIC; total current is more jagged.
- Additional hPIC/Vorpal comparisons for other sheath parameters are ongoing.



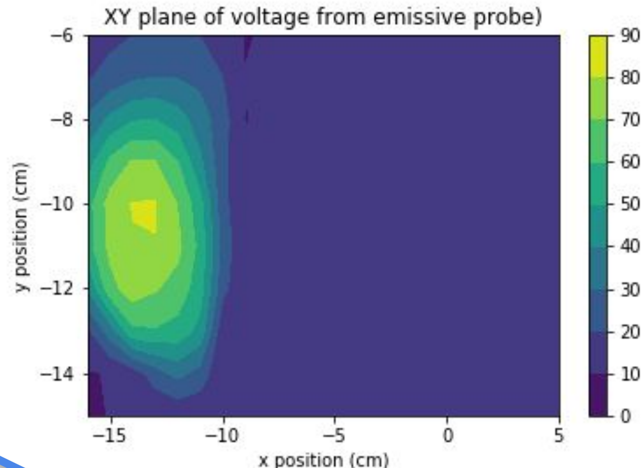
<eΦ/T_e> (6.98) is low relative to hPIC

Application of post-processing RF sheath model to LAPD

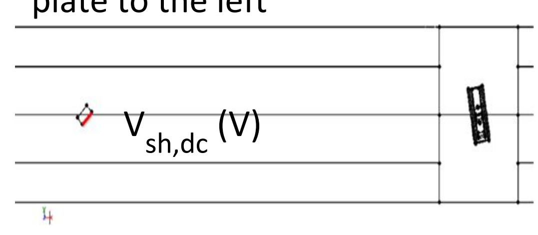
Post processing simulation result - DC sheath voltage distribution on the plate: thermal + RF rectified contribution.

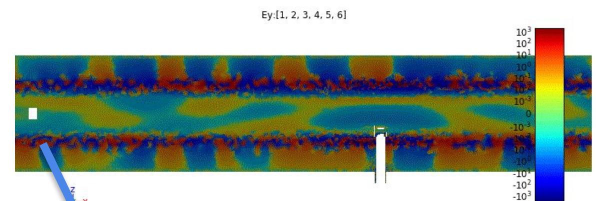


Experimental measurements of sheath on LAPD

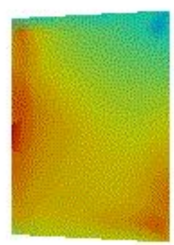


Model LAPD geometry with antenna to the right and target plate to the left

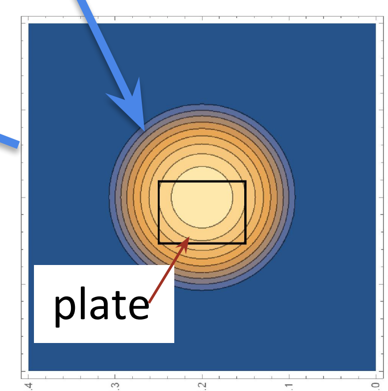




Simulation of core fast wave with slow waves in the edge.



RF B field perp to plate

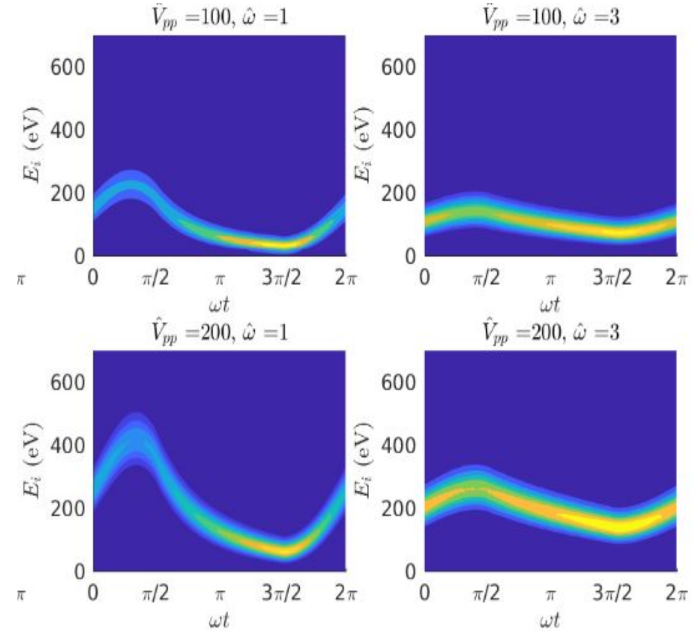


Post processing model is applied to simulation field results at the target plate to produce the DC rectified sheath voltage.

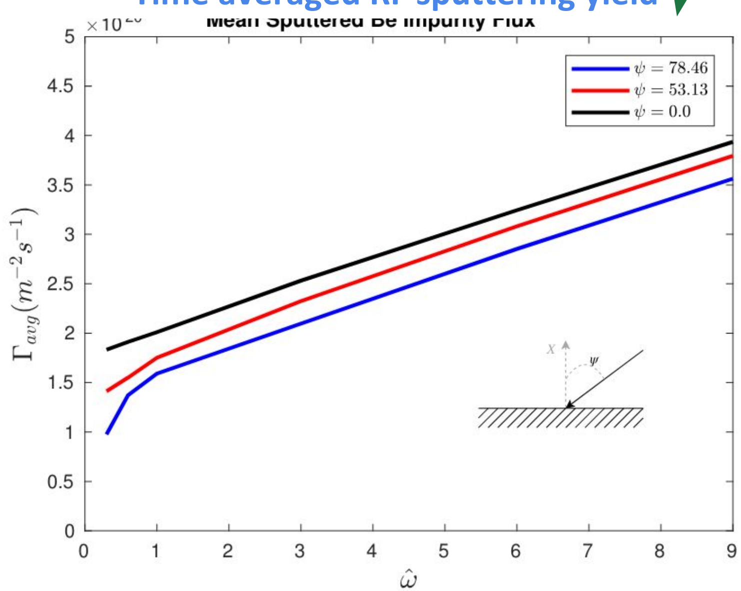
RF Sputtering model

- PMI code Fractal-Tridyn used to resolve the sputtering yield through an RF period.
- Time averaging gives a sputtering yield which can be used as impurity source on transport time scales.

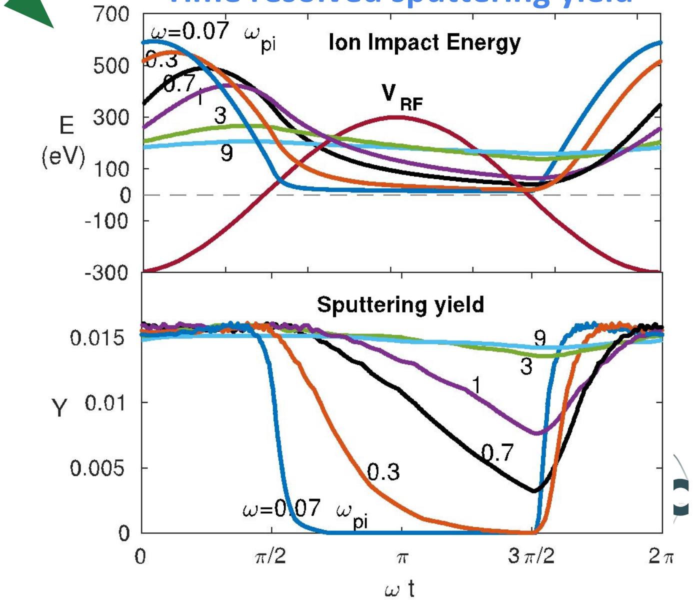
Time resolved RF induced ion impact energy



Time averaged RF sputtering yield



Time resolved sputtering yield



Summary - I

- **Hierarchy of high fidelity RF wave solvers for the fusion plasma edge are being developed**
  - MFEM based “mini app” wave solver (Stix Mini-App)
  - MFEM based full fidelity wave solver (Petra-M)
  - Treat complicated 3D edge / antenna geometry with linear / nonlinear BC’s (RF sheath)
  - Variety of pre-conditioner techniques (physics-based, algebraic) under investigation
- **Equilibrium & turbulent far-SOL transport is being treated in the presence of RF**
  - Braginskii fluid transport solver based on MFEM Mini App - includes anisotropy and complicated geometry of the far SOL
  - RF interaction with SOL turbulence is being studied with SOLT-3D (BOUT++) - includes effects of wave scattering and coupling to RF sheath and ponderomotive force

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Summary - II

- **3D FEM RF simulation model (Petra-M) is being deployed and validated. Applications thus far include**
  - LAPD HHFW antenna simulations
  - Full torus HHFW simulation for NSTX
  - ICRF antenna modeling for JET ITER-like antenna.

- **High fidelity studies of RF sheath and sputtering include**
  - Parameterization of a sub-grid RF sheath model
  - Benchmarking kinetic vs fluid sheath models (NoFlu, hPIC, Vorpal)
  - 1D, phase resolved (on the RF cycle) RF sputtering model (based on PMI code F-Tridyn)

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