Overview: Center for Simulation of Fusion Relevant RF Actuators

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

2018 Scientific Discovery through Advanced Computing (SciDAC-4) Principal Investigator Meeting

July 23-24, 2018
Rockville, MD

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

RF-SciDAC Center is a collaboration of FES and ASCR participants from DoE laboratories, universities, and private companies

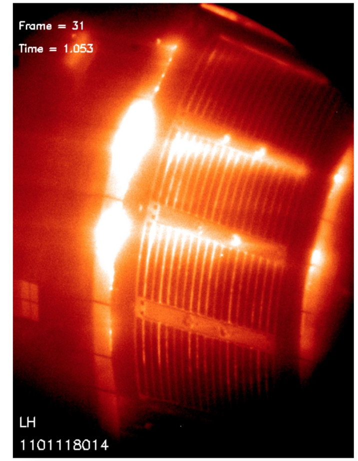
- **Massachusetts Institute of Technology**,
  - P. T. Bonoli, B. Biswas (**GS**), A. Ram, S. Shiraiwa, A. E. White, J. C. Wright
- **Oak Ridge National Laboratory**,
  - **FES:** D. L. Green, R. Barnett (**GS**), J. Lore, C. Lau, D. B. Batchelor (SC), L. A. Berry (SC)
  - **ASCR:** E. D'Azevedo, L. Mu
- **Princeton Plasma Physics Laboratory**
  - N. Bertelli, E.-H. Kim
- **Lawrence Livermore National Laboratory**
  - **FES:** A. Dimits, I. Joseph, T. Rognlien, M. Umansky
  - **ASCR:** T. Kolev, M. Stowell, V. Dobrev, Post-doctoral associate (TBD)
- **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, K. Karan (Post-doc)
- **University of Illinois - Urbana Champaign,**
  - D. Curreli, M. Elias (**GS**)

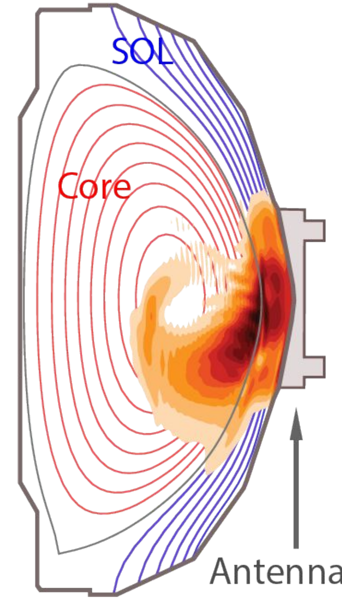
Outline

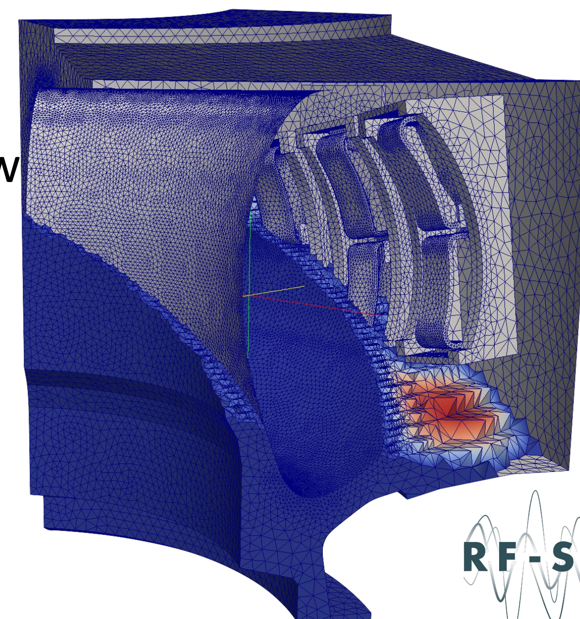
- Scientific goals of RF-SciDAC Center.
- Relationship to previous RF-SciDAC Center.
- Roles of applied mathematics and computer science in achieving scientific goals:
    - Identification of ASCR relevant project needs.
    - MFEM
    - PUMI
        - **Example application: RF + turbulence**
    - High fidelity driven scaling limits
    - Iterative methods
    - Non-linear boundary conditions
        - **Example application: Validation of non-linear sheath BC on LAPD.**
        - **Example application: Impurity generation from RF sheath.**
    - MFEM + PUMI based far-SOL transport solver.
- Relationship to other FES SciDAC centers.

Scientific objectives of the RF-SciDAC Project

- Develop an integrated simulation of the antenna + sheath + scrape-off-layer + core plasma system which fully utilizes leadership class computing.
- Move towards a quantitative predictive capability for the response of the plasma to RF power.
- Validate this predictive capability on appropriately diagnosed experiments.
- Work closely with the WDM Centers (AToM-SciDAC, TRANSP) to make both our new code development efforts, as well as the established hierarchy of RF tools, available within their environment.
- Use these tools to inform design of robust, impurity-mitigating RF heating and current drive sources for future fusion devices.

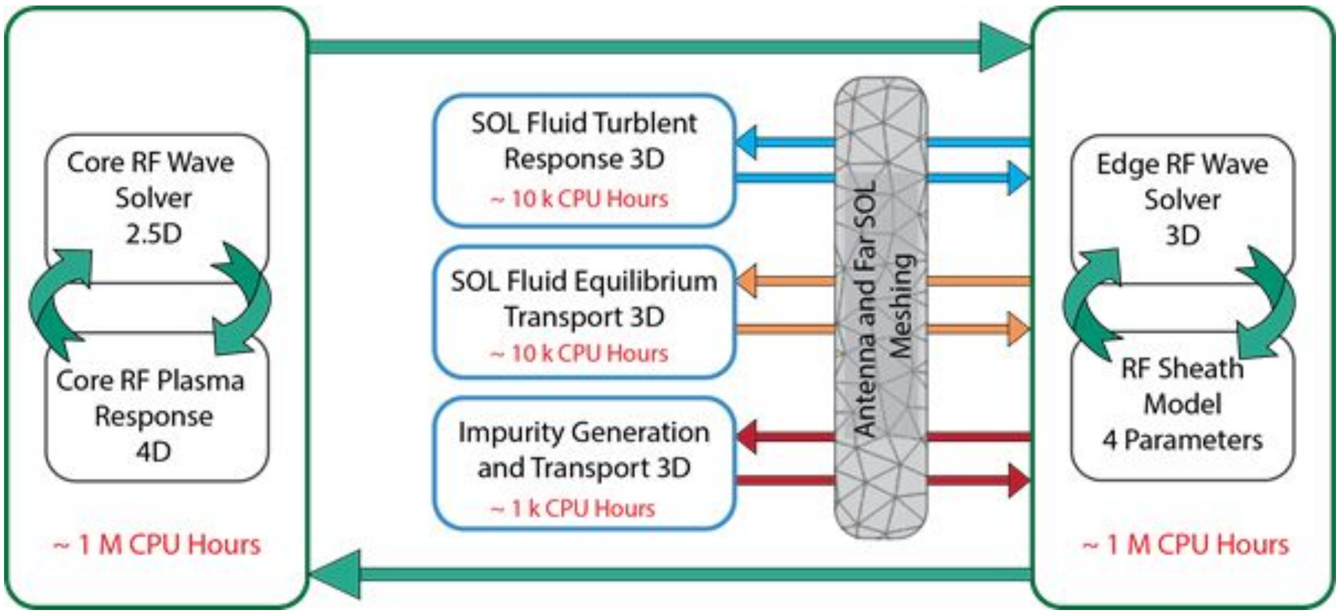






RF-SciDAC

Use simulation capability to predict the self-consistent interaction of RF power with the core plasma and 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 & 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) / T. Kolev (ASCR)
- **Thrust 4: RF + Impurity Generation**
    - J. Wright (FES) / D. Curreli (FES)
- **Relative breakdown of FES and ASCR resources:**
    - 76% - FES
    - 24% - ASCR

RF-SciDAC

One focus of the new center is to deliver the production core RF codes as WDM components.

- Completing WDM components for the existing RF hierarchy of core wave-particle interaction tools (Thrust 1).
  - Components and workflows utilize the AToM supported tools (See next talk by J. Candy):
    - Integrated Plasma Simulator (IPS) - a framework for HPC code integration.
    - OMFIT python tools.
- Also building RF integrated workflows to be provided to AToM
  - IPS-TorLH + IPS-CQL3D (Used in the 2017 DOE theory milestone).
  - **IPS-GENRAY + IPS-CQL3D (to be used by AToM - Park et al.).**
  - IPS-TORIC + IPS-CQL3D.
  - IPS-TORIC + IPS-P2F + IPS-NUBEAM.
  - Examples to be added to the ips-examples AToM repo https://github.com/ORNL-Fusion/ips-examples
- Verification, validation and application of these coupled workflows continues.

RF-SciDAC

Success of new scientific objectives relies heavily on applied mathematics and computer science expertise

- Quantitative prediction of the impact of RF power on the SOL plasma requires
  - High geometric fidelity.
  - Large 3D domain size (> 100M DoF)
  - Treatment of multiple RF wave scales.
  - Treatment of anisotropic heat and momentum transport in the far-SOL.
  - Coupling to kinetic core plasma response.
- In parallel to utilizing existing edge RF and SOL codes, we are developing the required capability based on ASCR tools:
  - **MFEM:** A scalable finite element method library
    - A new RF antenna edge code
    - A new far-SOL equilibrium and turbulent transport fluid solvers.
  - **Iterative solver techniques / preconditioners** are needed for global edge RF antenna simulations at > 100M DoF.
  - **PUMI:** Parallel unstructured meshing capabilities for simulating complicated antenna structures.

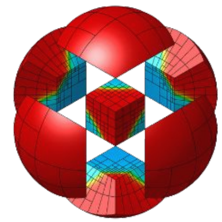
RF-SciDAC

MFEM

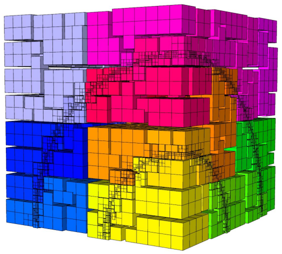
Lawrence Livermore National Laboratory

Free, lightweight, scalable C++ library for finite element methods. Supports arbitrary high order discretizations and meshes for a wide variety of applications.

- **Flexible discretizations on unstructured grids**
  - Triangular, quadrilateral, tetrahedral and hexahedral meshes.
  - Local conforming and non-conforming refinement.
  - High-order mesh optimization (ASCR Base).
  - Bilinear/linear forms for variety of methods: Galerkin, DG, DPG, …
- **High-order methods and scalability**
  - Arbitrary-order H1, H(curl), H(div)- and L2 elements. Arbitrary order curvilinear meshes.
  - MPI scalable to millions of cores. Enables application development on wide variety of platforms: from laptops to exascale machines.
- **Solvers and preconditioners**
  - Integrated with: HYPRE, SUNDIALS, PETSc, SUPERLU, …
  - Auxiliary-space AMG preconditioners for full de Rham complex.
- **Open-source software**
  - Open-source (GitHub) with thousands of downloads/year worldwide
  - Part of FASTMath, ECP/CEED, xSDK, OpenHPC, ...



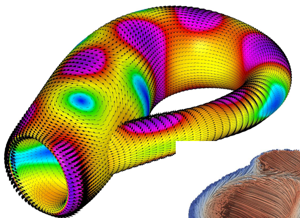
High order curved elements



Parallel non-conforming AMR

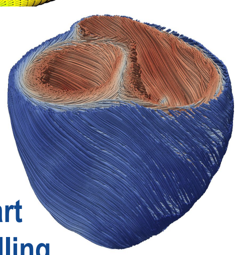
CEED EXASCALE DISCRETIZATIONS

FASTMATH

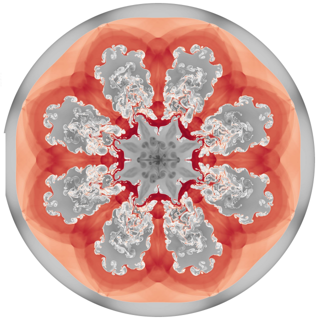


Surface meshes

ASC



Heart modelling



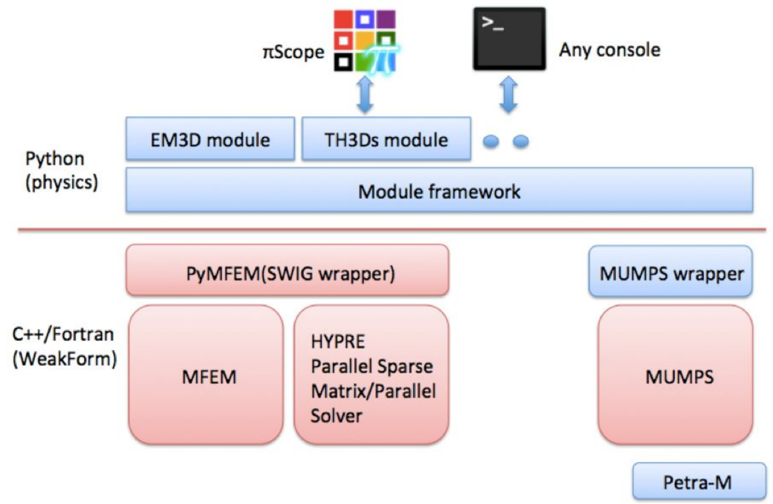
Compressible flow ALE simulations

http://mfem.org

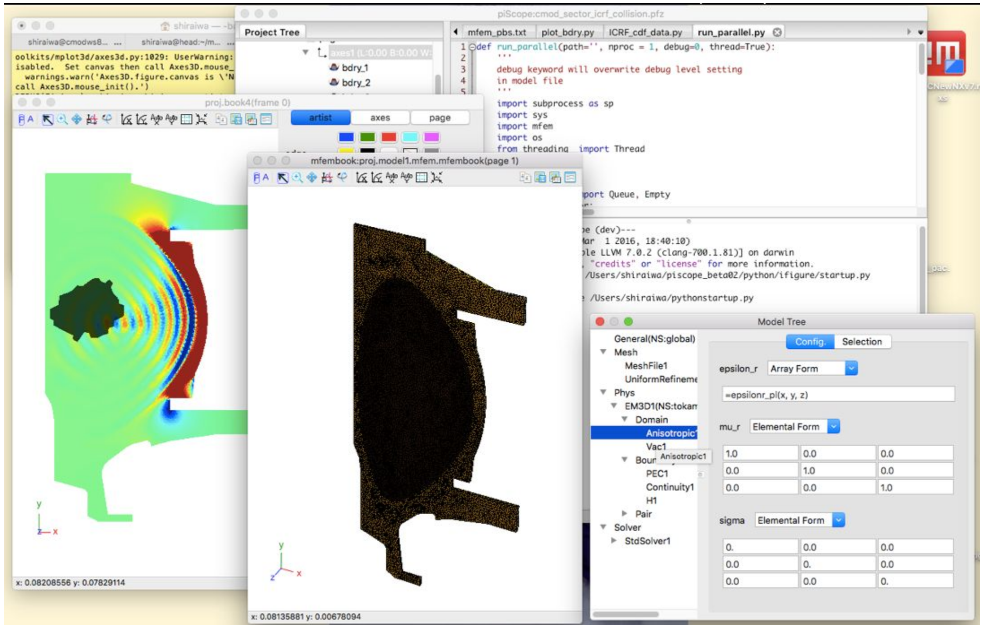
RF-SciDAC

Petra-M – Physics Equation Translator with MFEM

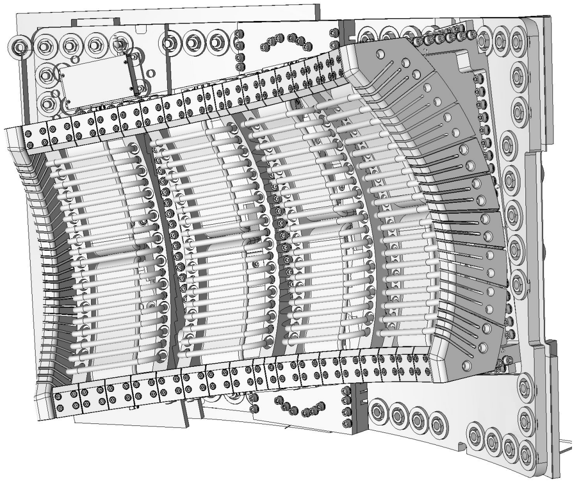
- Integrated FEM analysis environment using MFEM for the finite element library.



- Developed in close collaboration with the MFEM Team.
  - Here we use this for the edge, cold-plasma full-wave solver component.

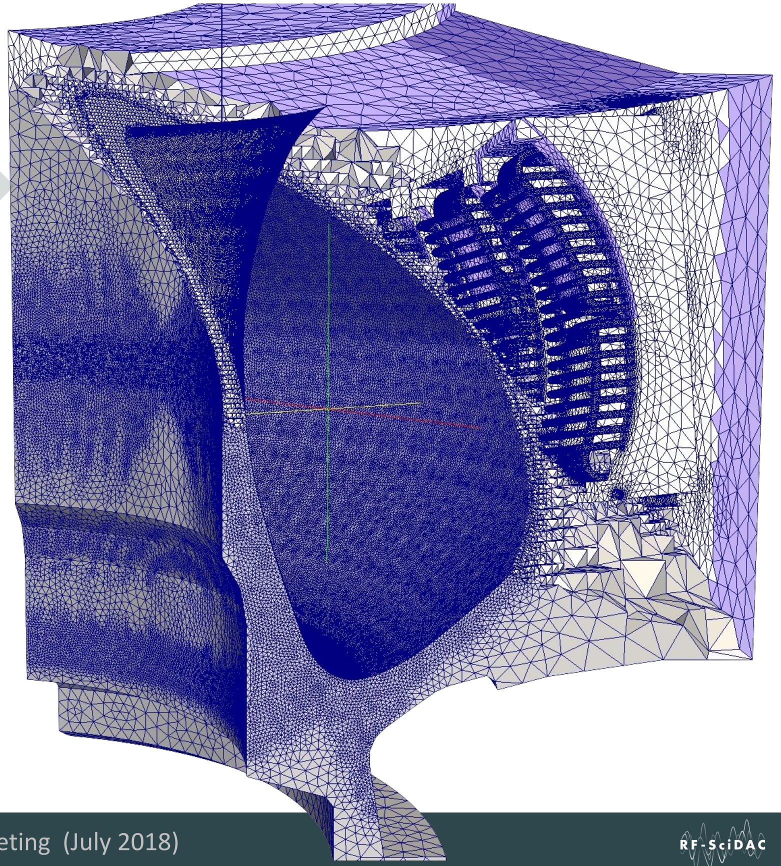


CAD model of antenna.



Quantitative RF predictions require high fidelity geometry and advanced meshing (PUMI)

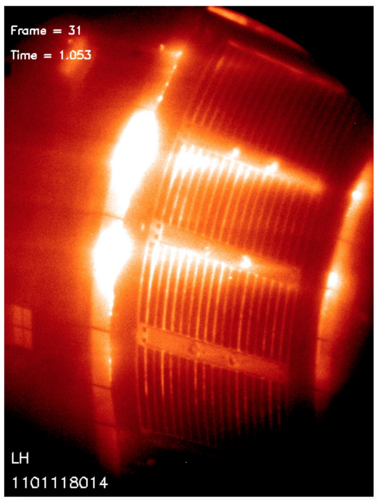
- Accurate RF simulations require
  - Detailed antenna CAD geometry.
  - Extract boundary curves from 2D magnetic geometry and convert it to 3D CAD model.
  - Analysis geometry combining CAD, physics geometry and faceted interfaces.



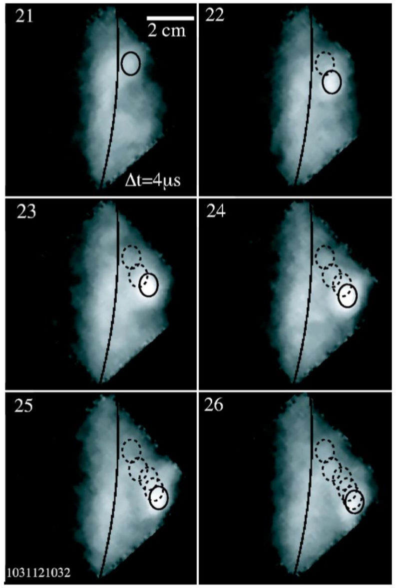
- Developments underway
  - Tools for combining and interacting with geometry from multiple sources.
  - Providing parallel curved mesh adaptation **integrated into MFEM.**
  - Integration into Petra-M.

How does the density perturbation in front of antenna impact RF wave propagation?

- Experiment shows field-line aligned density perturbations
  - Striation (stationary).
  - Turbulent blobs.

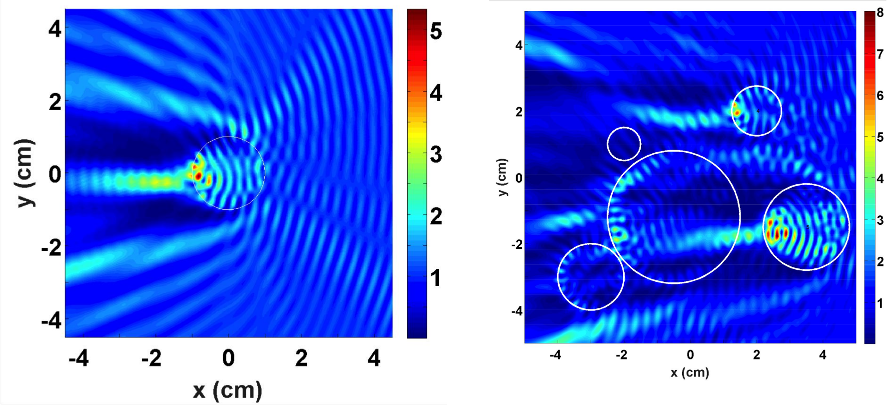


Glowing striations of LHCD Launcher [1]



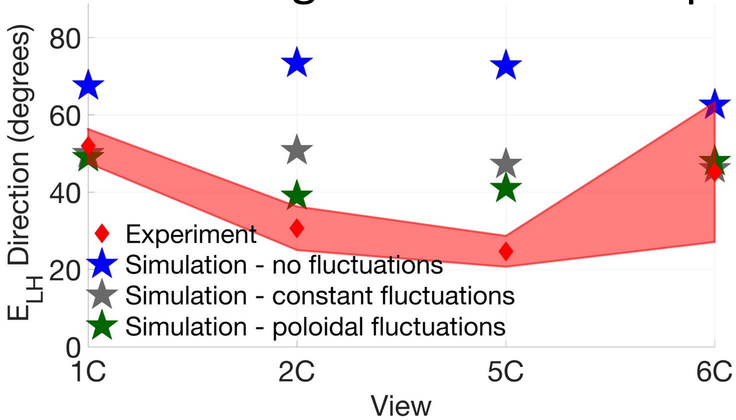
High speed movie of blob in SOL [2]

- Earlier simulation (in 2D) indicates the importance of density perturbation.



[Ram et al., PoP 2016; Ioannidis et al., PoP 2017;Valvis et al., JPP 2018; Bairaktaris et al., JPP 2018]

... and better agreement with expt.

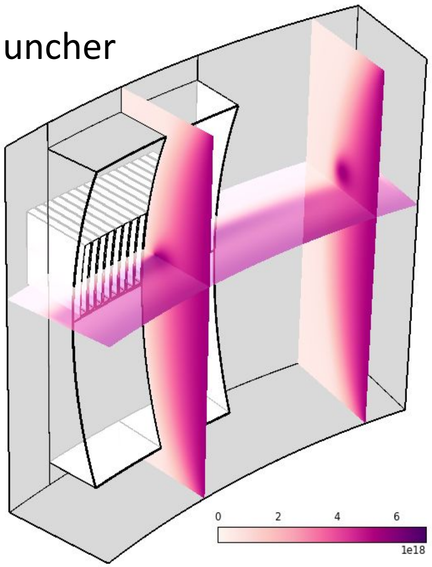


[1] O. Meneghini, et. al.,"Modeling Non-linear Plasma-wave Interaction at the Edge of a Tokamak Plasma", (2011)
[2] J. L Terry. et. al., "High speed movies of turbulence in Alcator C-Mod", RSI, (2004)

True 3D LH wave simulation indicates that the LH wave field pattern could be significantly altered

LH resonance-cone propagation is largely destroyed.

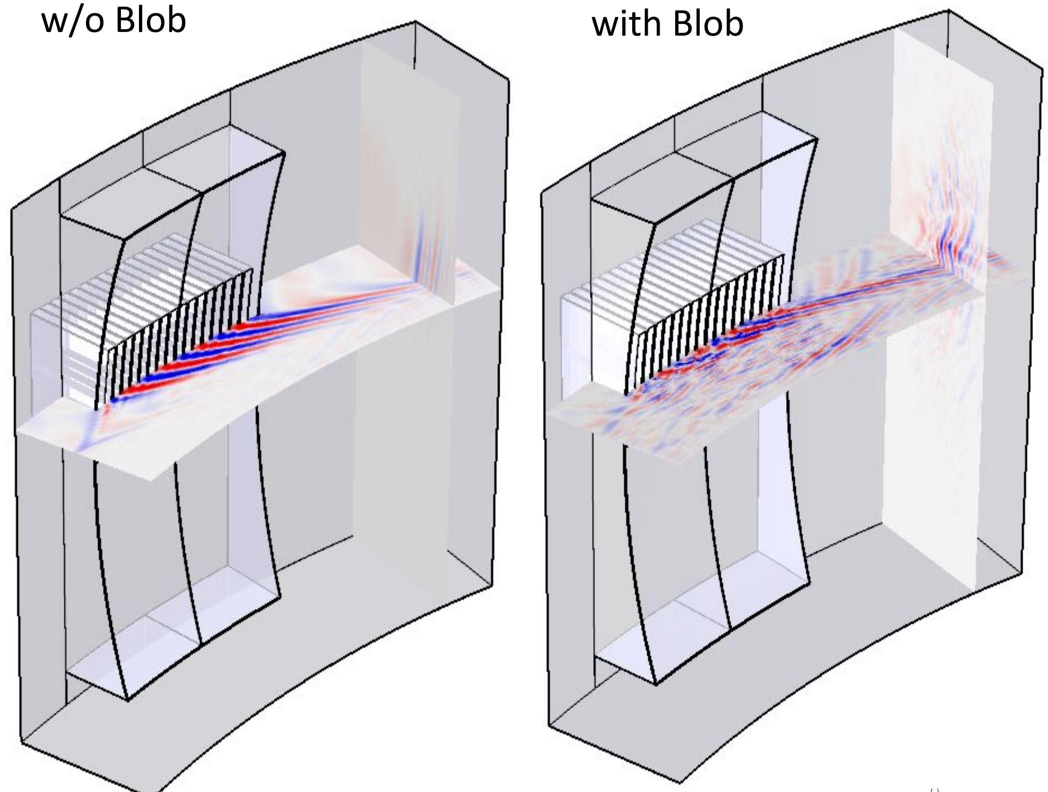
LH launcher



$E_{toroidal}$ of 4.6 GHz LH wave propagation

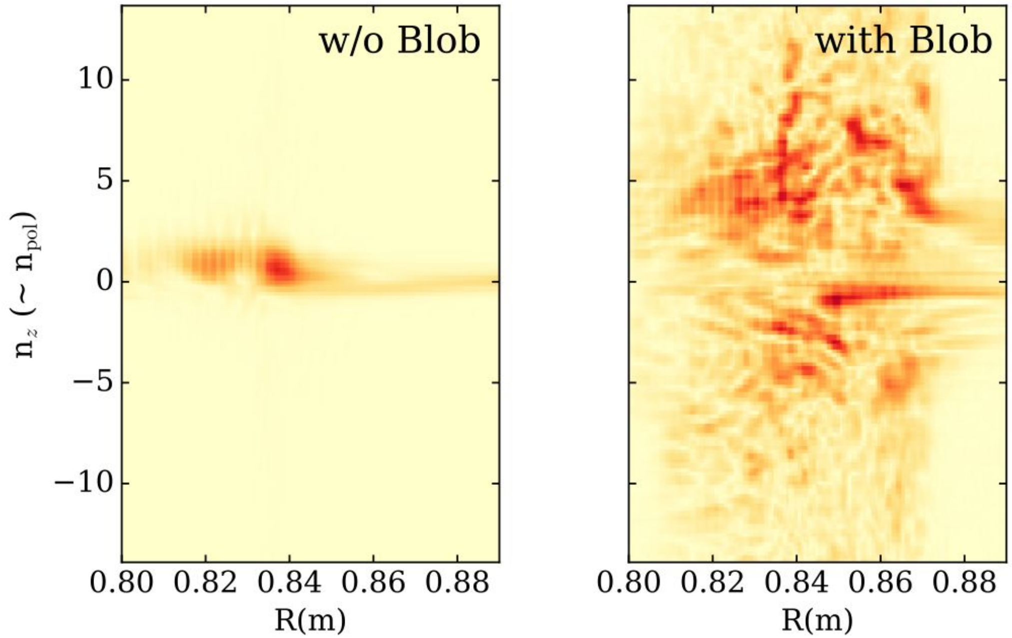
w/o Blob

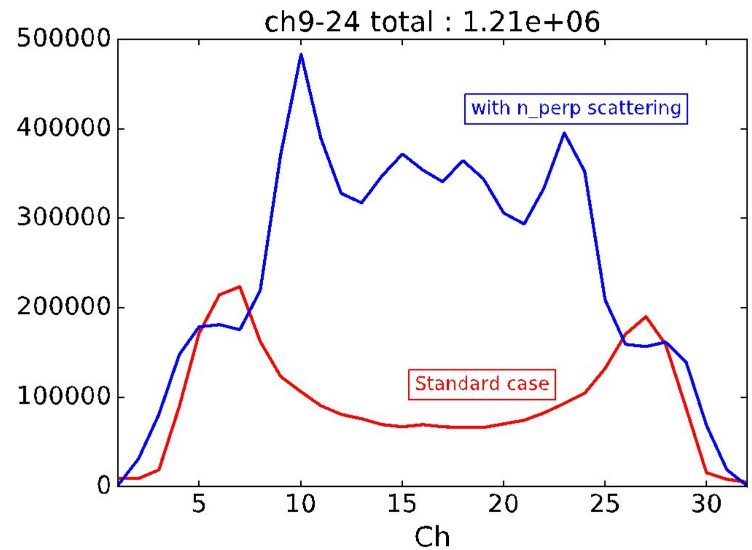
with Blob



Field aligned density modulation placed in front of LH launcher. The modulation was computed by solving the diffusion from particle source in front of the launcher.

Wave spectral broadening of the vertical wave number has significant impacts on core wave propagation





Perpendicular wavenumber spectrum is broadened with the blob.

LHCD simulation (GENRAY/CQL3D) using the broadened spectrum predicts...

- More peaked HXR emission profiles (in better agreement with experiment).
- Total driven current increased due to the synergistic interaction among scattered waves.

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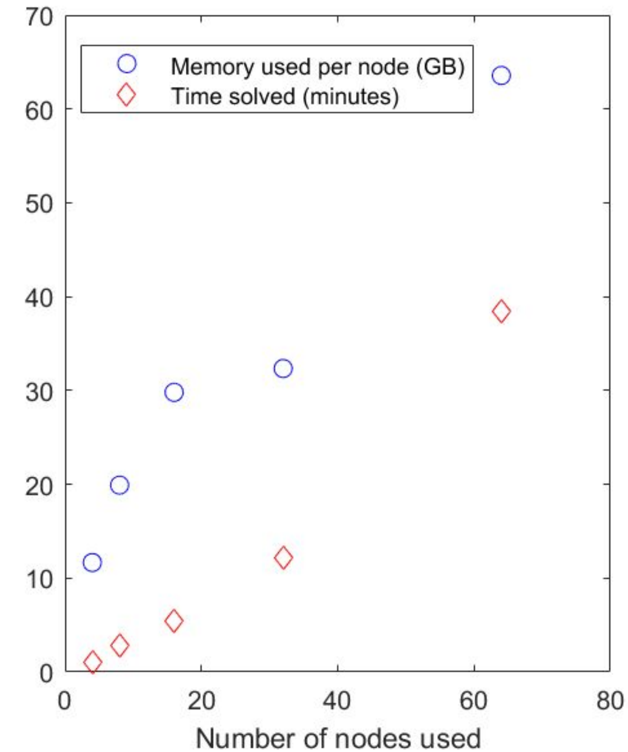
High fidelity means a need for iterative methods

- High fidelity 3D requirements have revealed the **limitations on traditional sparse direct solvers**.
  - For large N > 10^6 , storage for LU factorization can be O(100) times that of the original matrix, i.e., **prohibitively high cost in memory.**
  - While increasing the number of nodes (for a fixed problem size) provides more memory, it results in less work per node and increased communication.
  - MUMPS also demonstrates a base per-node memory footprint proportional to problem size.

3-D weak scaling (DoF/node ~ 0.25 M)



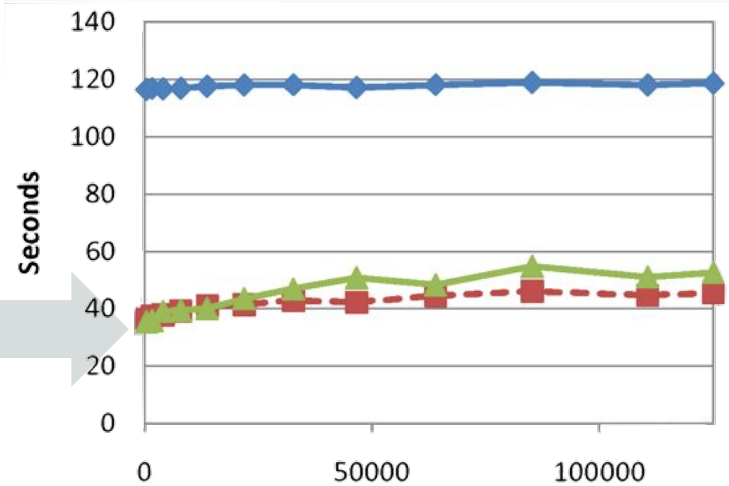
Iterative approaches are being investigated

- Iterative methods will be required to solve frequency domain RF equations at the desired fidelity. Approaches include ...
  - AMS (within hypre), which requires additional fine-grid information, that MFEM can generate and pass automatically.
  - Preconditioners based on physics insights and intuition.
  - Reformulation of curl curl with elliptic operator.

$$-\nabla \times \nabla \times \mathbf{E} + \frac{\omega^2}{c^2}\mathbf{E} = -\imath\omega\mu_0 \mathbf{J}_{\mathrm{ext}}$$

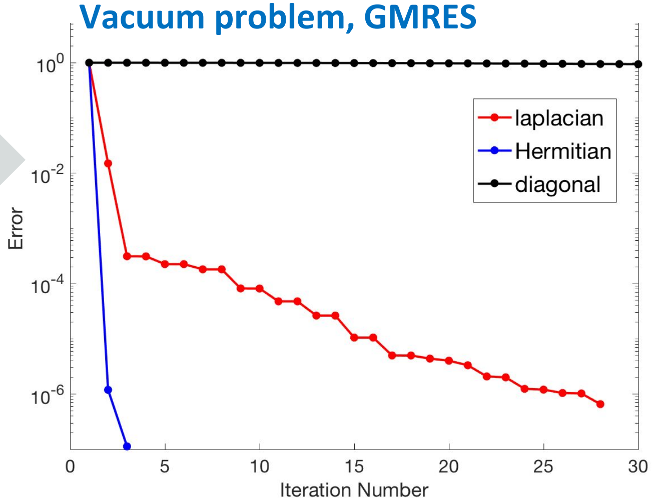
$$-\nabla \times (\nabla \times \mathbf{E}) = \nabla^2 \mathbf{E} - \nabla(\nabla \cdot \mathbf{E})$$

AMS weak scaling example (MFEM)*.

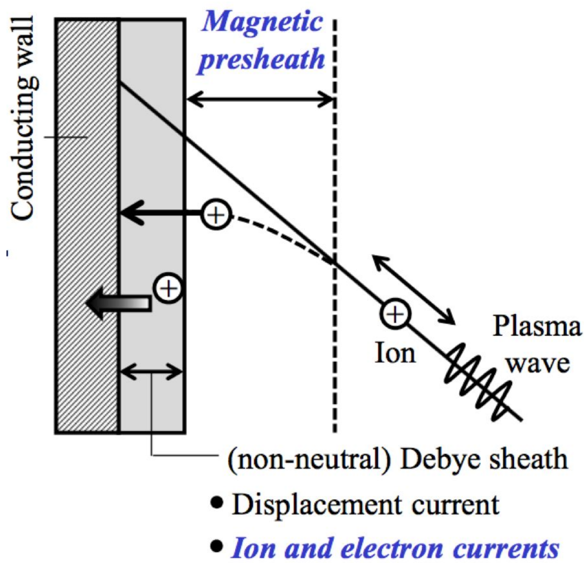


* Tz. Kolev, P. Vassilevski, “Parallel auxiliary space AMG for H(curl) problems”, JCM

Vacuum problem, GMRES



Iterative methods are also required for the Finite Element Formulation of non-linear Sheath BCs



$$\boxed{\mathbf{E}_t^{(\mathrm{pl})} = -\nabla_t V_{\mathrm{RF}}}$$

$$\boxed{V_{\mathrm{RF}} = -J_n^{(\mathrm{sh})} z_{\mathrm{sh}} = -\frac{\omega}{i} D_n^{(\mathrm{pl})} z_{\mathrm{sh}}}$$

Coupled Eqs.

1) RF wave field determines the displacement, thus the RF sheath voltage.
2) Gradient of RF sheath voltage determines the boundary condition for RF electric field.

Frequency Maxwell: solve for $\vec{E}, \vec{J}$ in H(Curl;Ω)

$$\nabla\times\left(\mu^{-1}\nabla\times\vec{E}\right) - \omega^2\epsilon\vec{E} = i\omega\vec{J} \quad \text{in } \Omega$$

subject to: $\hat{n}\times\left(\vec{E}\times\hat{n}\right) = \hat{n}\times[(-\nabla\varphi)\times\hat{n}]$ on $\Gamma \equiv \partial\Omega$,

$\varphi \equiv \alpha\,\hat{n}\cdot\left(\epsilon\vec{E}\right)$ in H(Grad;Γ)

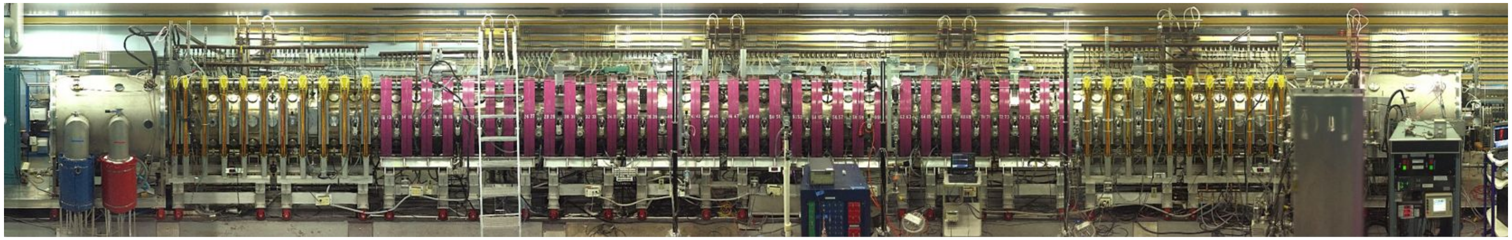
Weak form with *auxiliary field* $\vec{D}$ in H(Div;Ω):

$$\left(\mu^{-1}\nabla\times\vec{E}, \nabla\times\vec{W}\right)_\Omega - \left(\omega^2\epsilon\vec{E}, \vec{W}\right)_\Omega + \langle\vec{\lambda}, \vec{W}\rangle$$
$$+ \langle\vec{E}, \vec{u}\rangle + (\nabla\varphi, \vec{u})_\Gamma + (\varphi, v)_\Gamma - \left(\alpha\hat{n}\cdot\vec{D}, v\right)_\Gamma$$
$$+ \left(\vec{D}, \vec{F}\right)_\Omega - \left(\epsilon\vec{E}, \vec{F}\right)_\Omega = \left(i\omega\vec{J}, \vec{W}\right)_\Omega$$

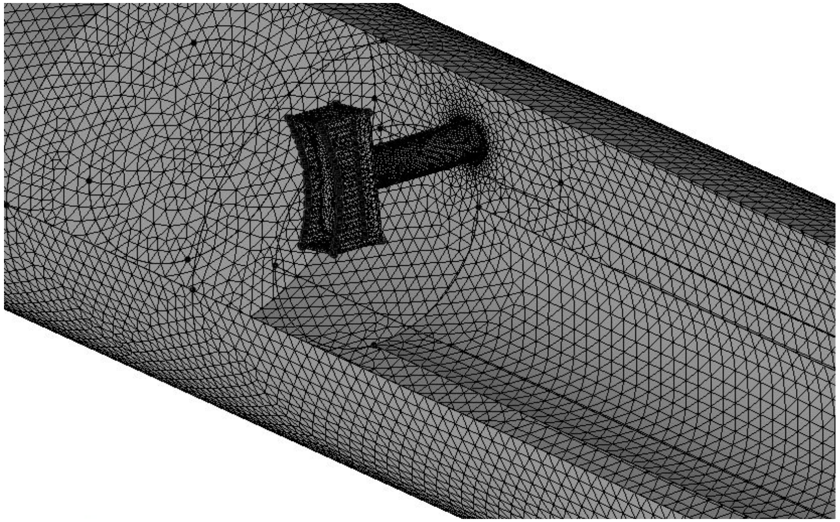
$\vec{W}$ in H(Curl;Ω), $\vec{\lambda}$, $\vec{u}$ in H(Curl;Γ), $\vec{F}$ in H(Div;Ω),

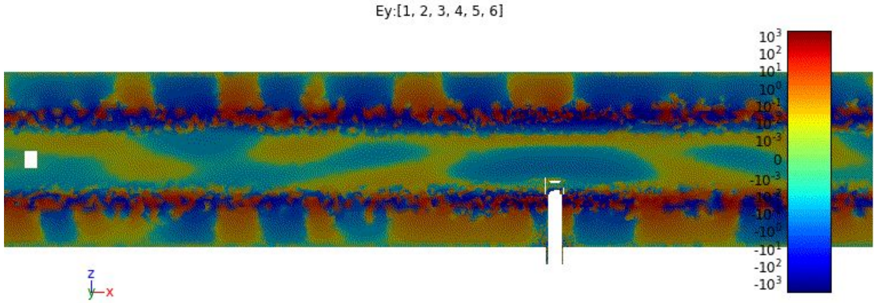
v in H(Grad;Γ), $\langle\cdot,\cdot\rangle$ is duality pairing between Ω, Γ

LAPD device for sheath model validation



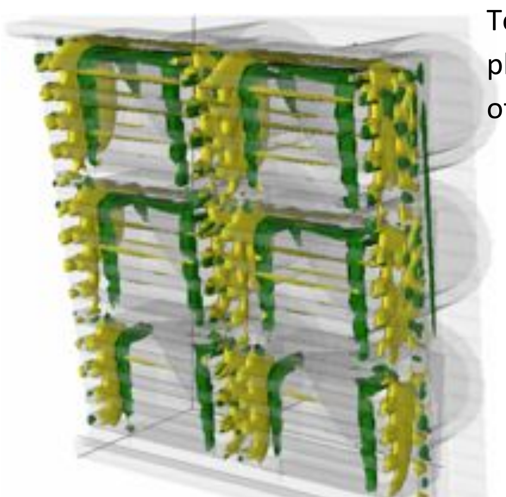
- LAPD (LArge Plasma Device at UCLA)
  - Simple geometry with reproducible, accessible plasmas; ideal for validating sheath predictions.
  - 18 m plasma column.
  - 15 ms plasma pulse at 1 Hz.
  - Plasma similar to tokamak edge with $n_e \sim 10^{19}\ m^{-3}$, $T_e \sim 10$ eV.
  - Low magnetic field ~ 1000 G.
  - 100 kW, 2.38 MHz, 1 ms pulse single strap antenna.
- Modeling
  - Mesh entire 18 m column with antenna, limiters and RF target plate.
  - Apply post processing sheath model.
  - S=0, P=0 resonant surfaces seen; slow wave near edge, fast wave near core.
  - Waves incident on plate angled at 45°, mode conversion to slow wave ensues.
  - Fast wave propagates down device to strike target plate.





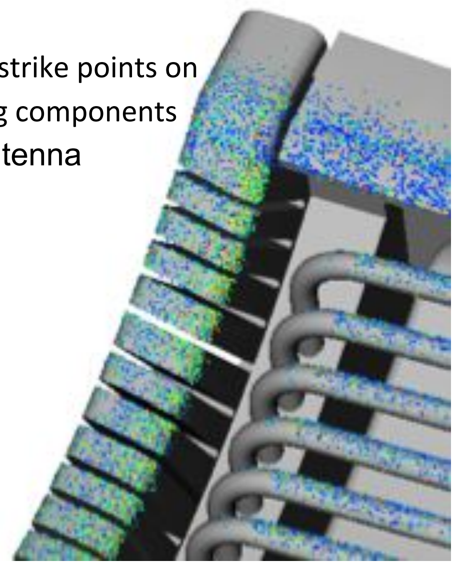
Sheath and impurity sputtering modeling with Vorpal

- Vorpal (VSim) – electromagnetic/electrostatic PIC code, finite-difference time-domain (FDTD) methods, kinetic (Boris) particles, expanding GPU capabilities, good parallel scaling up to 100k+ cores (OLCF, NERSC).
- Implementing sub-grid sheath boundary conditions using explicit local PIC modeling of the sheath*. This capability includes implementations of ...
  - Particle flux to surfaces, with particle energies adjusted to reflect passage of test particles through the sheath potential drop.
  - Erosion and surface heat loads.
  - Sputtering models** for plasma-facing surfaces.

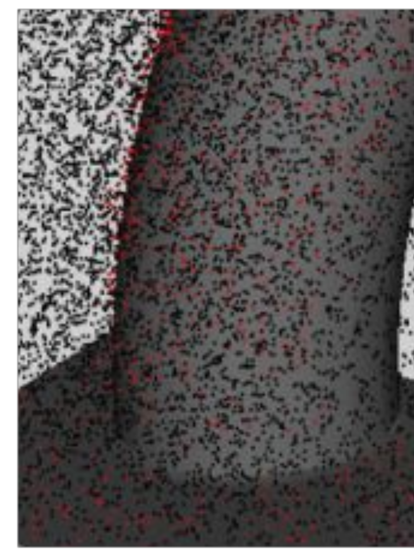


Sheath potential on surfaces of ITER ICRF antenna module

Test-particle strike points on plasma-facing components of C-Mod antenna



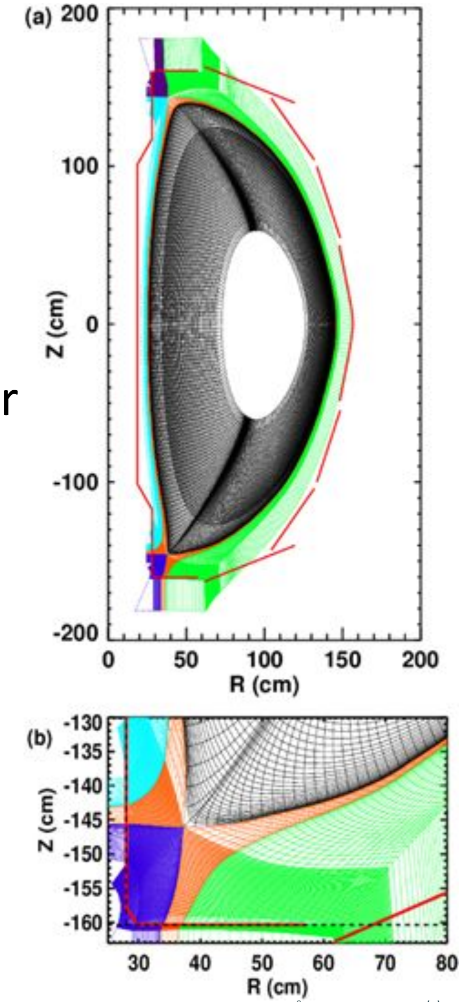
Sputtered high-Z neutral atoms (red) from antenna surface, arising from ion-wall collisions



* T. G. Jenkins & D. N. Smithe, PSST **24**, 015020 (2015), J. R. Myra, PoP **24**, 072507 (2017)
** Y. Yamamura & H. Tawara, At. Data Nucl. Data Tables 62, 149 (1996)

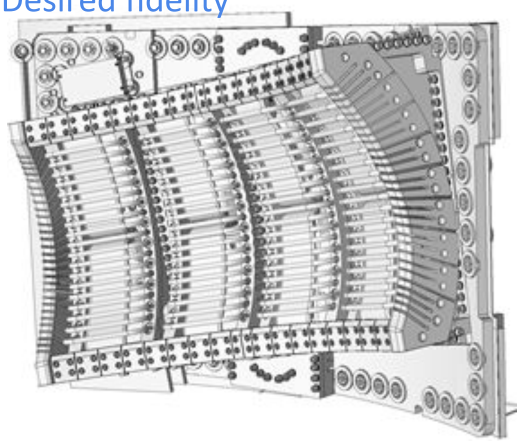
Existing far-SOL fluid transport solvers have limitations on fidelity and physics

Example of typical PFC fidelity.

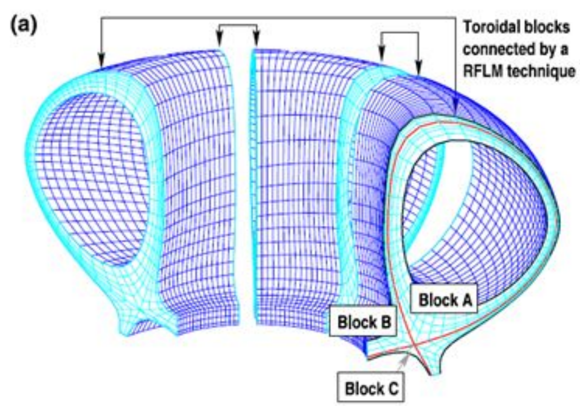


- EMC3-EIRENE solves steady-state 3D fluid transport equations using field-aligned mesh.
- Grid can extend radially to antenna structure and PFC structure.
- EMC3 scales to 100s of cores, possible improvements under investigation.
- Meshing can be challenging due to structured grid requirements.
  - Results in a large memory footprint.

Desired fidelity

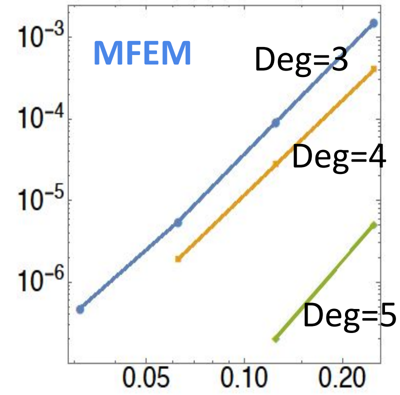


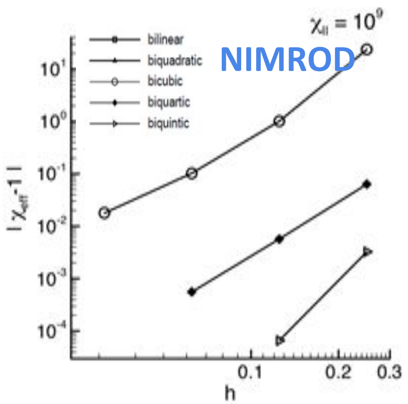
Extruded in 3D via RFLM method.

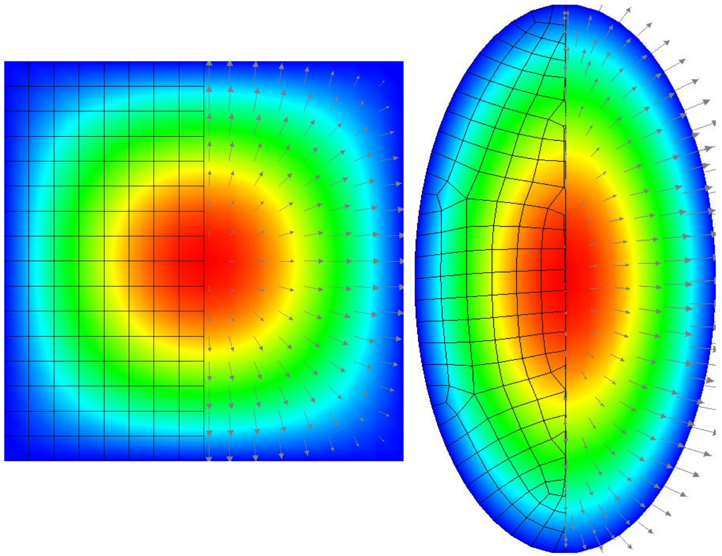


Far-SOL MFEM-based solver on non-field-aligned mesh is being investigated

- EMC3-EIRENE widely used to model 3D equilibrium transport code in tokamaks/ stellarators, but meshing can be challenging
  - We need both high geometric fidelity to match RF antenna structures, and high-order basis functions to capture the large anisotropy (~10^3 - 10^9) in heat transport in the SOL
- Using MFEM and advanced meshing tools may provide us both.
- **High order:** Implemented NIMROD benchmarks
  - Anisotropic transport problem with analytic solution to assess error (numerical diffusion)
- Tested Cartesian (non-aligned) grid using MFEM
  - Demonstrates acceptable error at challenging anisotropy level

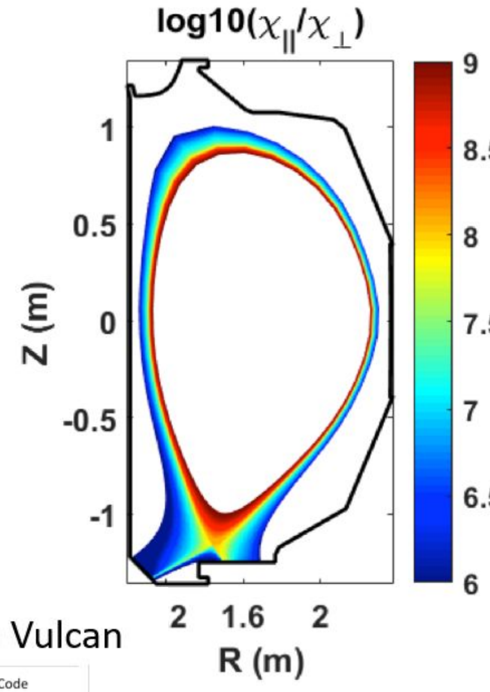


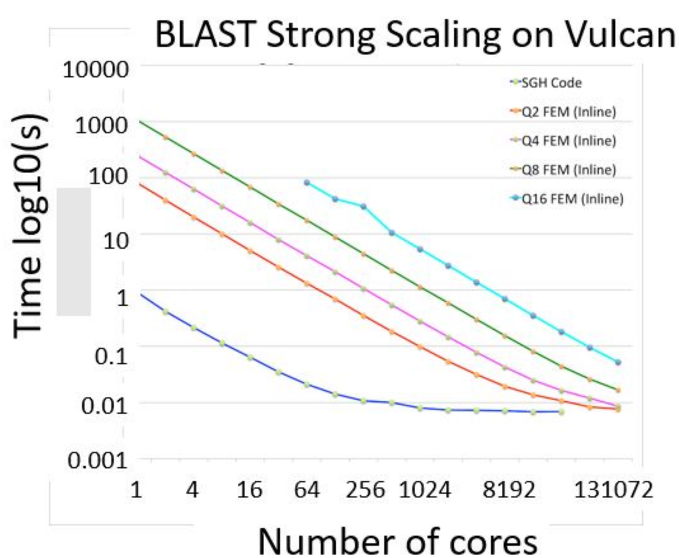




Far-SOL MFEM-based solver on non-field aligned mesh is being investigated

- Advanced Meshing
  - Since the edge plasma has lower ratio of parallel to perpendicular diffusivity, the best method may be a grid that transitions from field-aligned in near-SOL to PFC-aligned at wall.
  - Apply advanced meshing techniques (RPI meshing center).
- High Order Scaling
  - MFEM's high order methods show promising scaling on modern computer architectures (both CPU and GPU).





RF-SciDAC

RF SciDAC-4 Center interacts with other FES SciDAC Centers in the following areas

- Fusion Energy Sciences SciDAC-4 efforts are targeting components for a fusion Whole Device Model (WDM).
- This Center will provide a hierarchy of RF heating and current drive components to the WDM effort.
- Interactions with the following centers are being discussed or are ongoing …
  - AToM-SciDAC and TRANSP whole device modeling Projects
    - Providing RF components and workflows (and using coupling technologies).
  - TDS-SciDAC and SCREAM-SciDAC Centers
    - Investigation of RE mitigation by Whistler waves.
  - Edge Simulation Laboratory (ESL) and HBPS-SciDAC Center
    - Long term goal of coupling to kinetic SOL simulation.
  - PSI-SciDAC Center
    - F-TRIDYN and GITR codes for sputtering and trace impurity tracking.

RF - SciDAC

End