SciDAC Center for Fusion Relevant RF Actuators: Overview, RF Scattering from Turbulence, and Overcoming Scaling Limits for High Fidelity Predictive Simulation.

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

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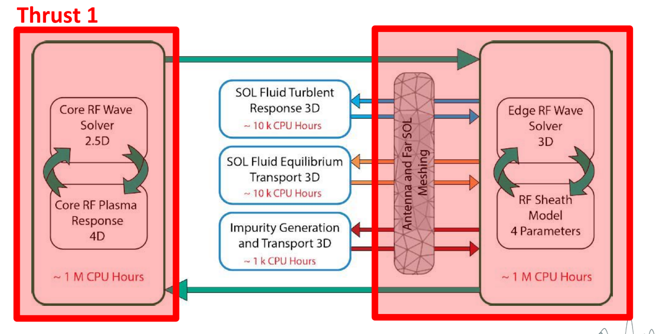
Scientific Objectives & Organization of the RF-SciDAC Project

- **Develop an integrated simulation for quantitative prediction of the antenna + sheath + scrape-off-layer + core plasma system which fully utilizes leadership class computing.**
- Validate this predictive capability on appropriately diagnosed experiments including dedicated RF test stands, linear devices, and existing tokamaks.
- Project organized into 4 thrusts:
  - Thrust 1: RF WDM Components & Thrust Common Efforts **(this poster)**
  - Thrust 2: RF + Turbulence **(this poster)**
  - Thrust 3: RF + Equilibrium Transport **(other poster)**
  - Thrust 4: RF + Impurity Generation **(other poster)**
- **Use these tools to inform design of robust, impurity-mitigating RF heating and current drive sources for future fusion devices.**

Thrust 1: Production RF WDM components, interaction with AToM / TRANSP & thrust common developments.



Codes available as WDM components and core-edge coupling

- Production (ready for integration)
  - GENRAY https://github.com/compxco/genray.git
  - AORSA https://github.com/ORNL-Fusion/aorsa
  - TORIC / TORIC-HHFW / TORLH https://code.ornl.gov/jcwright77/toric5-ornl
  - P2F https://github.com/ORNL-Fusion/p2f
  - CQL3D https://github.com/compxco/cql3d.git
- Development
  - RF Monte Carlo code (under initial design).
  - Petra-M … for the high geometric fidelity, cold, edge plasma solver https://github.mit.edu/shiraiwa/PetraM_Base
  - MFEM compatible meshing capability for RF structures.
- Project wide effort to improve software engineering best practices to enable code longevity.

Integration with AToM and TRANSP via the "Integrated Plasma Simulator" (IPS)

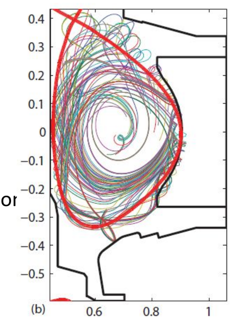
- Our center is making the hierarchy of RF tools available via the AToM-SciDAC supported integration technologies (IPS & OMFIT).
- The IPS is a ASCR+FES developed file-based framework enabling serial and/or parallel simulation codes to function interoperably by providing a flexible capability for integrated, multi-physics simulation.
- Collaboration with AToM has seen GENRAY being used to demonstrate how to incorporate a component into IPS.
- Support & improve the RF components in TRANSP.
  - TORIC including non-Maxwellian multi-species.
  - Verify / compare FPP and CQL3D.
  - Verification of RF kick operator implemented in NUBEAM.
  - GENRAY for EC waves & MPI GENRAY (in collaboration with CompX base theory effort).

Delivery production RF codes as WDM components, both for AToM and RF-SciDAC.

- Completing IPS components for the existing RF hierarchy of core wave-particle interaction 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 immediately 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
- Verify RF and RF+SOL components.
- Validation and application of these components continues.

GENRAY & CQL3D

- **GENRAY:** Ray tracing code.
  - Used for different RF frequency regimes
  - Include a SOL model.
  - Include a scattering model from density fluctuation
- **CQL3D:** Fokker-Planck code.
  - Used for different RF frequency regimes
  - Coupled to GENRAY, TORIC & AORSA
- Present activities
  - Recently made available on GitHub.
  - Constructing new IPS modules utilizing the updated AToM tools.
  - Parallel performance of GENRAY being investigated and optimized.



Ray trajectories for LH waves in C-Mod

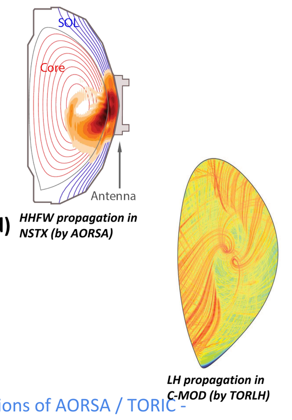
AORSA, TORIC and TORLH

Core plasma, full-wave tools.

- **AORSA (ion-cyclotron frequency range)**
  - Pseudo-spectral.
  - Dense matrix inversion.
  - AORSA includes also SOL plasma.
  - Coupled to CQL3D via IPS.
- **TORIC (ion-cyclotron) / TORLH (lower-hybrid)**
  - Finite-difference + spectral.
  - Block-sparse matrix inversion.
  - Coupled to MFEM for cold edge.
  - Coupled to CQL3D via IPS.

Present activities

- Public repo for AORSA now available.
- Investigating single-node, no communication versions of AORSA / TORIC perhaps for use as preconditioners.
- Exploring preconditioner for iterative solver to replace sparse direct solver.
  - Sparse direct method is not scalable for large 3D problems so finding effective preconditioner for iterative solver is important.
- Modernizing IPS workflows for inclusion in AToM.



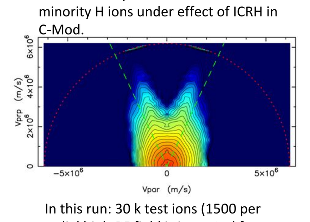
HHFW propagation in NSTX (by AORSA)

LH propagation in C-MOD (by TORLH)

A performance portable RF Monte Carlo code is required to future proof the hierarchy of RF tools.

- Legacy RF Monte-Carlo tools (e.g., ORBIT-RF, NUBEAM, etc) are difficult to include in high-performance integrated workflows.
- Performance portability options (e.g., Kokkos, OpenMP4, OpenACC) are under investigation.
- Present activities (CompX, ORNL, …)
  - A simple Fortran demonstration code has been constructed to communicate the algorithm.

Example output of demonstration code: a steady-state distribution of minority H ions under effect of ICRH in C-Mod.



In this run: 30 k test ions (1500 per radial bin); RF field is imported from AORSA. Distribution is at the midplane position R=75 cm, not far from the ICR layer at R~68 cm.

Versatile FEM analysis frontend is being developed and has been applied to a variety of RF propagation modelings

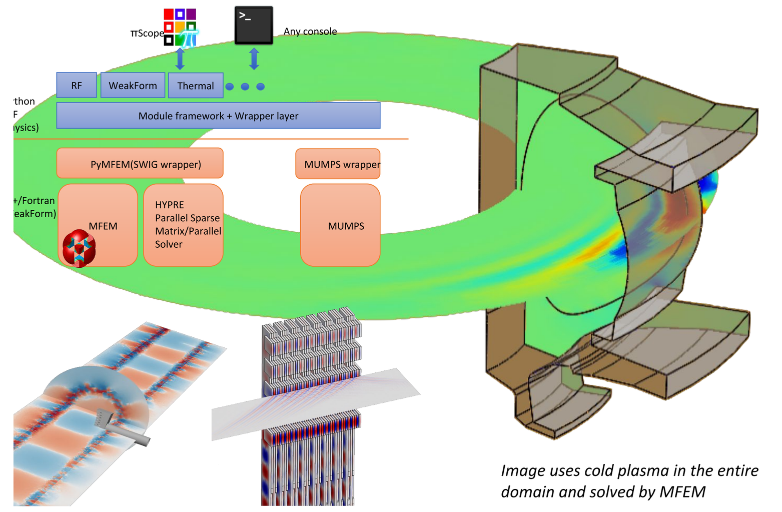
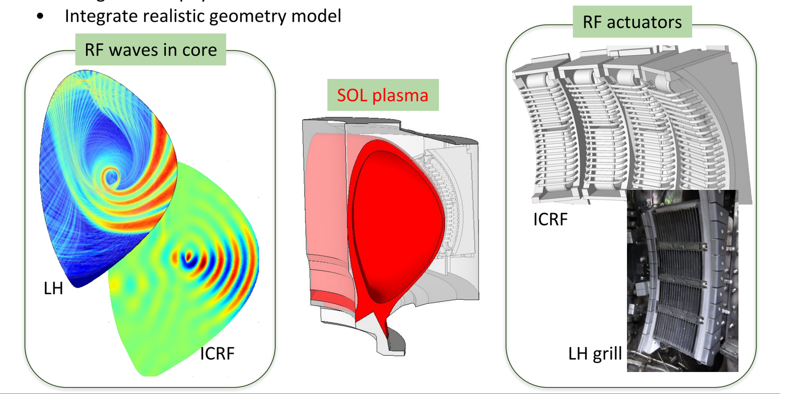


Image uses cold plasma in the entire domain and solved by MFEM

High fidelity RF simulation requires integrated approach

- Integrate Core/edge wave propagation/absorption
- Integrate with SOL plasma transport/turbulence
- Integrate PMI physics
- Integrate realistic geometry model



Scalable high quality mesh generation integrated into simulation workflow

Geometry elements from original source

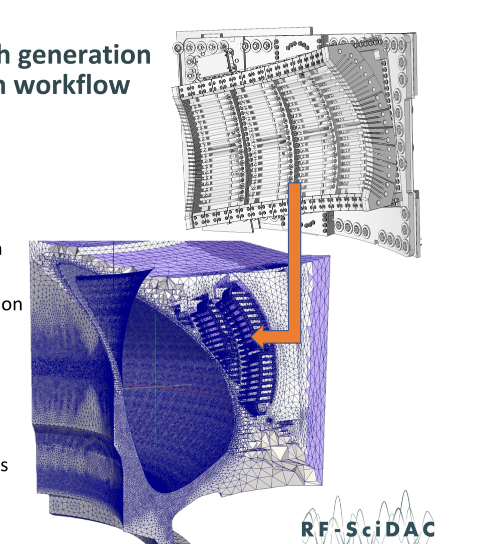
- Directly defeaturing CAD assemblies (with Simmetrix SimModeler)
- EFIT curves/core RF solver mesh

Curved mesh generation

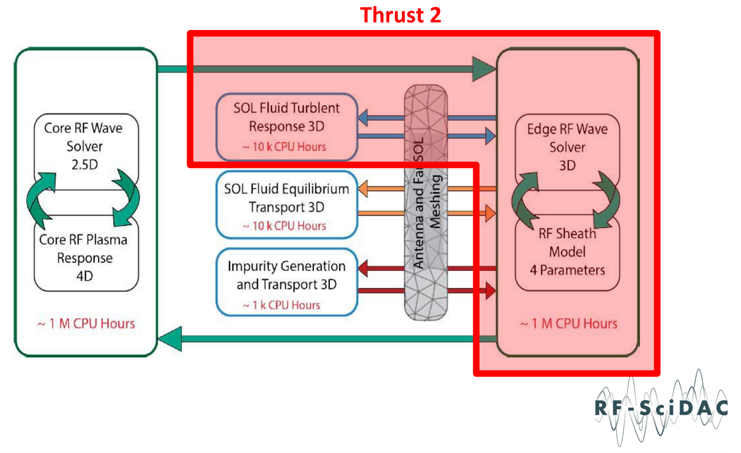
- Accurate geometry representation with a fewer elements

Integration into workflow

- MFEM : In-memory integration with parallel PUMI meshes (Simmetrix mesh loaded into PUMI)
- Integration into frontend-tools is in preparation (PetraM/πScope)



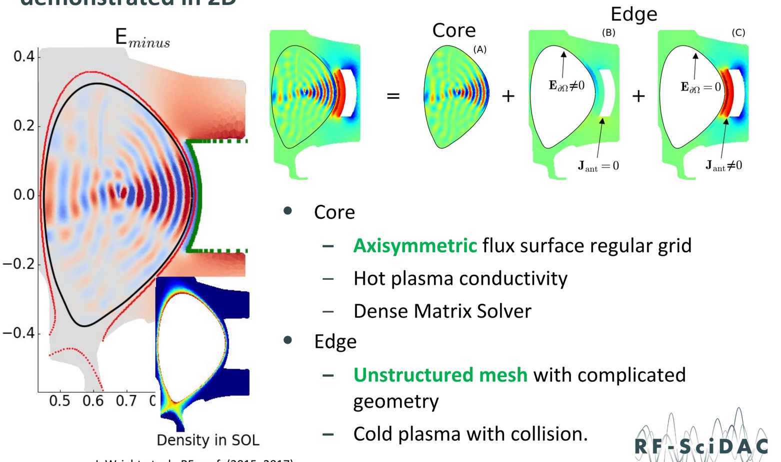
Thrust 2 : RF-Turbulence Interaction Component & Coupling Development



RF-turbulence interactions are important for understanding RF

- Turbulence affects RF propagation
  - Turbulent transport affects the mean density profile -> affects RF propagation, launcher coupling, and RF-sheath interactions
  - Large-amplitude filaments (="blobs") and resistive drift-wave fluctuations can scatter RF
- RF and associated launching structures affect turbulence
  - RF sheaths can directly seed instabilities
  - RF sheaths and ponderomotive forces result in flows
  - These can
    - stabilize turbulence (e.g., via shear flow)
    - or destabilize (e.g., via Kelvin-Helmholtz drives)

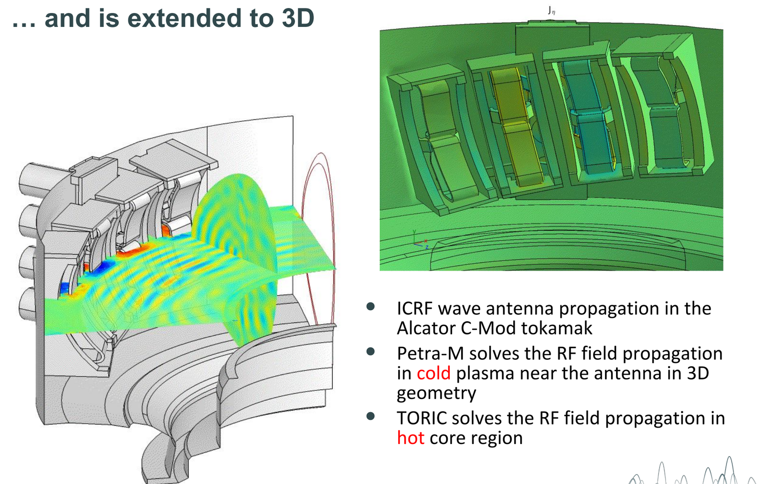
Core-edge integration of linear wave propagation is demonstrated in 2D



- Core
  - Axisymmetric flux surface regular grid
  - Hot plasma conductivity
  - Dense Matrix Solver
- Edge
  - Unstructured mesh with complicated geometry
  - Cold plasma with collision.

J. Wright et. al., RF conf. (2015, 2017)
S. Shiraiwa et. al, et al. N.F. (2017))

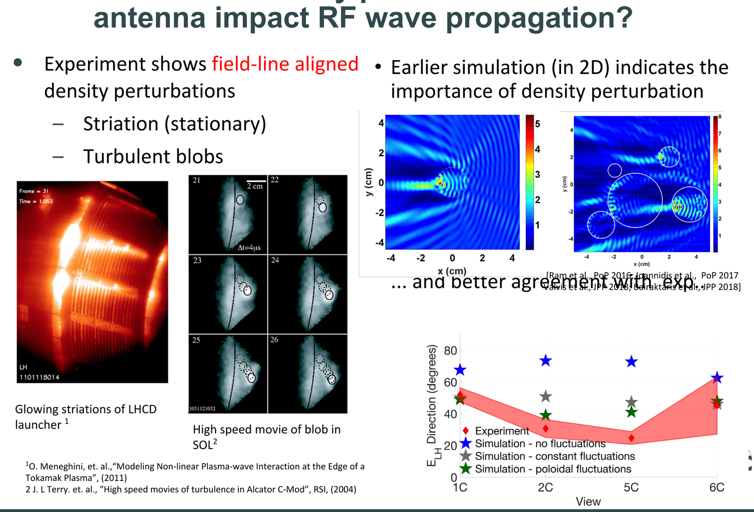
… and is extended to 3D



- ICRF wave antenna propagation in the Alcator C-Mod tokamak
- Petra-M solves the RF field propagation in cold plasma near the antenna in 3D geometry
- TORIC solves the RF field propagation in hot core region

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

- Experiment shows field-line aligned density perturbations
  - Striation (stationary)
  - Turbulent blobs
- Earlier simulation (in 2D) indicates the importance of density perturbation



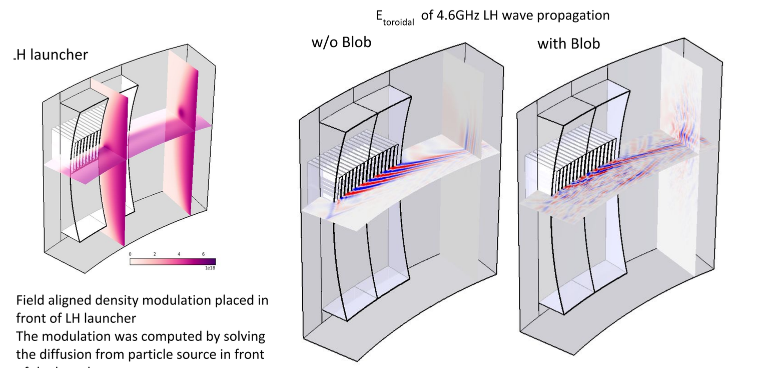
Glowing striations of LHCD launcher [1]

High speed movie of blob in SOL[2]

… and better agreement with exp.

[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)

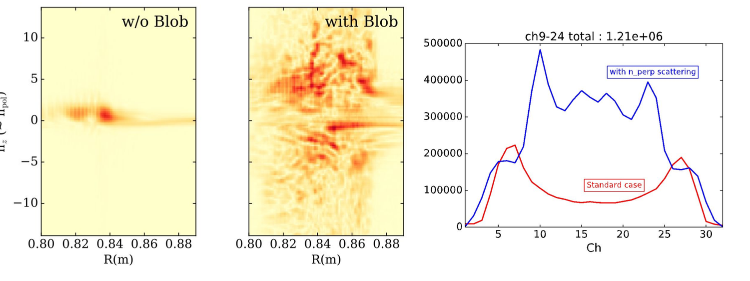
True 3D LH wave simulation indicates that the LH wave field pattern could be significantly altered



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

LH resonance-cone propagation is largely destroyed

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

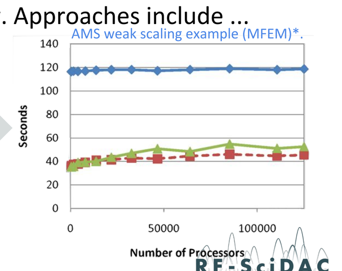


Perpendicular wavenumber spectrum is broadened with the blob.
LHCD simulation (GENRAY/CQL3D) using the broadened spectrum predicts…

- More peaked HXR emission profiles
- Total driven current increased due to the synergistic interaction among scattered waves.

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.**
- 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 problem with elliptic operator.
- Investigations into these approaches are underway.



Future work

BOUT++ turbulence model

- Exercise nonlinear terms
- Multi-region (core and SOL) model via appropriate BC's
- RF-sheath biased-plate BC on part of outer flux surface
  - 2D – verify against UEDGE
  - 3D rectangle
  - Impinging structure with fields from RF codes
- Ponderomotive force terms in turbulence model

RF Scattering models and simulations

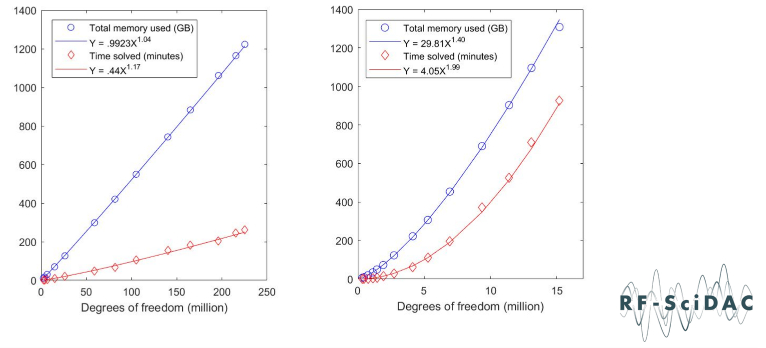
- Extend scattering simulations to used turbulent fields from BOUT/BOUT++ simulations
- Implement for other RF codes (GENRAY VORPAL)
  - Common data API for passing turbulent fields to RF codes

IPS wrapper + "example"

- First, run a BOUT++ model
- Then, couple this with RF code(s) using above API

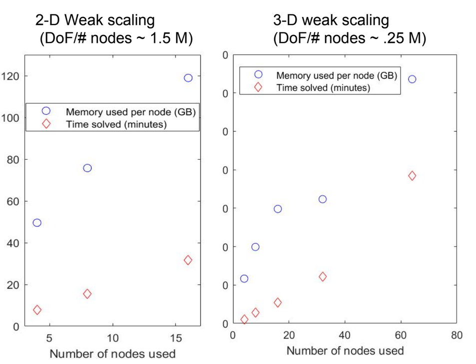
2-D and 3-D direct solvers on shared memory system is consistent with theoretical scaling

- a 1.5 TB cluster was used to solve 2-D and 3-D cold plasma problem
- memory and time used is approximately consistent with theoretical expectation
- Time to solve large 3-D problems can be expensive



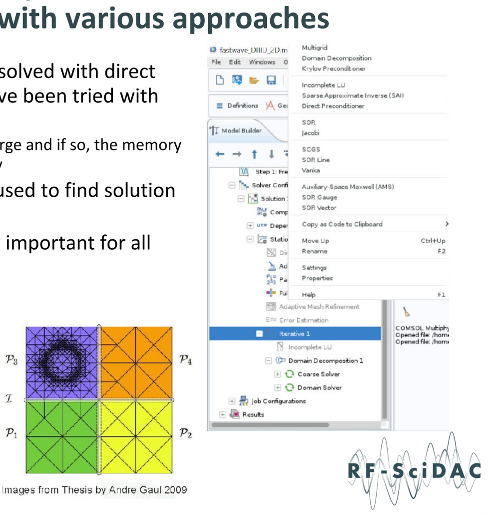
2-D and 3-D direct solvers on distributed memory system may be limited by memory per node

- MUMPS solver may be limited by memory per node (http://www.association-aristote.fr/Fichiers-2014/20-mai/04-C-Puglisi-Amestoy.pdf)
- COMSOL/MUMPS solver on cold plasma problem show similar trend
- Can iterative solvers also help with this issue?



Testing domain decomposition and other iterative solvers have started with various approaches

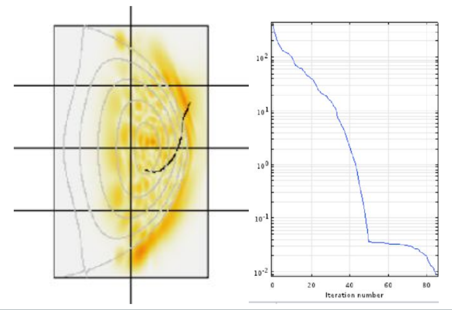
- Same cold plasma problem solved with direct solver on previous slides have been tried with iterative solvers in COMSOL
  - Test if iterative solvers converge and if so, the memory and time resources necessary
- Krylov methods are widely used to find solution x_k in Span{r,Ar,A^2r, A^3r …}
- Good preconditioner is very important for all iterative solvers
- Domain decomposition of each subdomain can be assigned to each processor independently, making distributed computing very efficient



Images from Thesis by Andre Gaul 2009

Convergence has proven difficult with domain decomposition with multiplicative Schwartz being the only relatively fast convergence

- GMRES with domain decomposition, multiplicative Schwartz, coarse domain was the only one that converged reasonably quickly to the direct solver answer
- above worked reasonably well for 2-D and 3-D ICRF cases tested so far
- No significant memory or time advantage on shared memory cluster



- other domain decomposition (additive Schwartz), multigrid, Krylov preconditioner etc. were very difficult to converge
- testing continues with plans focus on larger problems and distributed memory systems soon

Iterative Approaches to Wave Equations

- 3D sparse direct solver for N by N matrix
- Develop effective preconditioner for iterative methods
- Initial investigation in Matlab

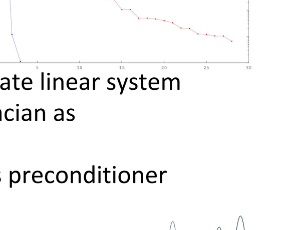
Preconditioner for Wave equation

- Curl of the curl can be split as

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

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

- Matlab application for 1D problem to generate linear system
- Simple vacuum problem to test vector Laplacian as preconditioner in GMRES(30)
- Note Hermitian part of matrix is effective as preconditioner

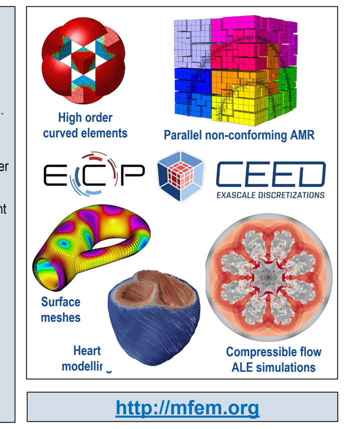


MFEM

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.
  - Bilinear/linear forms for variety of methods: Galerkin, DG, DPG, …
- **High-order and scalable**
  - 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.
- **Built-in solvers and visualization**
  - Integrated with: HYPRE, SUNDIALS, PETSc, SUPERLU, …
  - Accurate and flexible visualization with VisIt and GLVis
- **Open-source software**
  - LGPL-2.1 with thousands of downloads/year worldwide.
  - Available on GitHub. Part of ECP's CEED co-design center.



http://mfem.org

H(curl) diffusion is difficult to solve

EM diffusion modeled by second order definite Maxwell

$$\nabla\times\alpha\nabla\times E+\beta E=f\quad\mapsto\quad A_h x=b$$

Challenging due to large "near-nullspace":

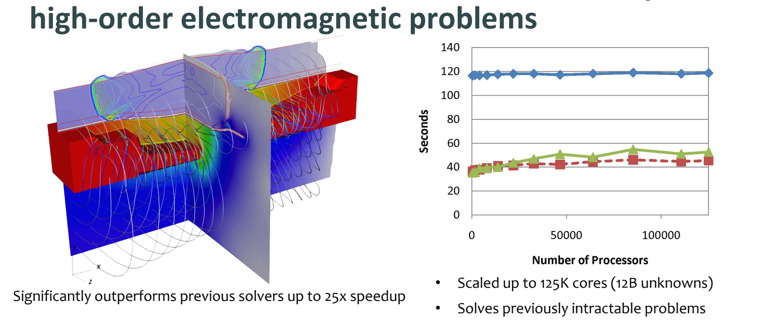
The Auxiliary-space Maxwell Solver (AMS) achieves scalability by reduction to the nodal subspaces

$$B_h = R_h + G_h B_{v,h} G_h^t + \mathbf{\Pi}_h \boldsymbol{B}_{\boldsymbol{v},h} \mathbf{\Pi}_h^t$$

Point smoother for A_h — AMG solver for $G_h^t A_h G_h$ — AMG solver for $\mathbf{\Pi}_h^t A_h \mathbf{\Pi}_h$

AMS a top 10 breakthrough in 2008 ASCR base report

AMS has been used on low-order and recently high-order electromagnetic problems

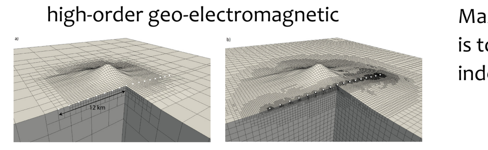


Significantly outperforms previous solvers up to 25x speedup

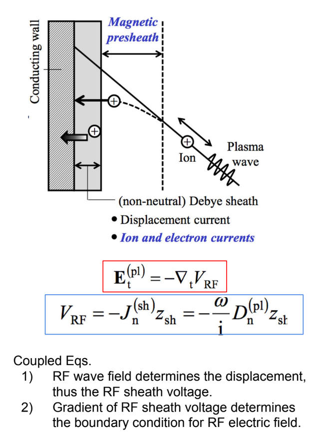
- Scaled up to 125K cores (12B unknowns)
- Solves previously intractable problems

Recent application of AMS to high-order geo-electromagnetic

AMS has been used for definite Maxwell's equations only, and plan is to test AMS on the cold plasma indefinite Maxwell's equation



Finite Element Formulation of Sheath BCs



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

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

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)

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

subject to: $\hat{n}\times(\vec{E}\times\hat{n})=\hat{n}\times[(-\nabla\varphi)\times\hat{n}]$ on $\Gamma\equiv\partial\Omega$, $\varphi\equiv\alpha\,\hat{n}\cdot(\epsilon\vec{E})$ in H(Grad;Γ)

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

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

$\vec{W}$ in H(Curl;Ω), $\vec{\lambda}$, $\vec{u}$ in H(Curl;Γ), $\vec{F}$ in H(Div;Ω), v in H(Grad;Γ), ⟨·,·⟩ is duality pairing between Ω, Γ