MODELING PLASMA DISCHARGE CLEANING OF SRF CAVITIES

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Tech-X and this Project

- Tech-X Corporation: 35 person company located in Boulder, CO
- Specialize in physics simulation software development and research
  - Electromagnetics, photonics, plasma discharges, fusion plasmas, microwave devices

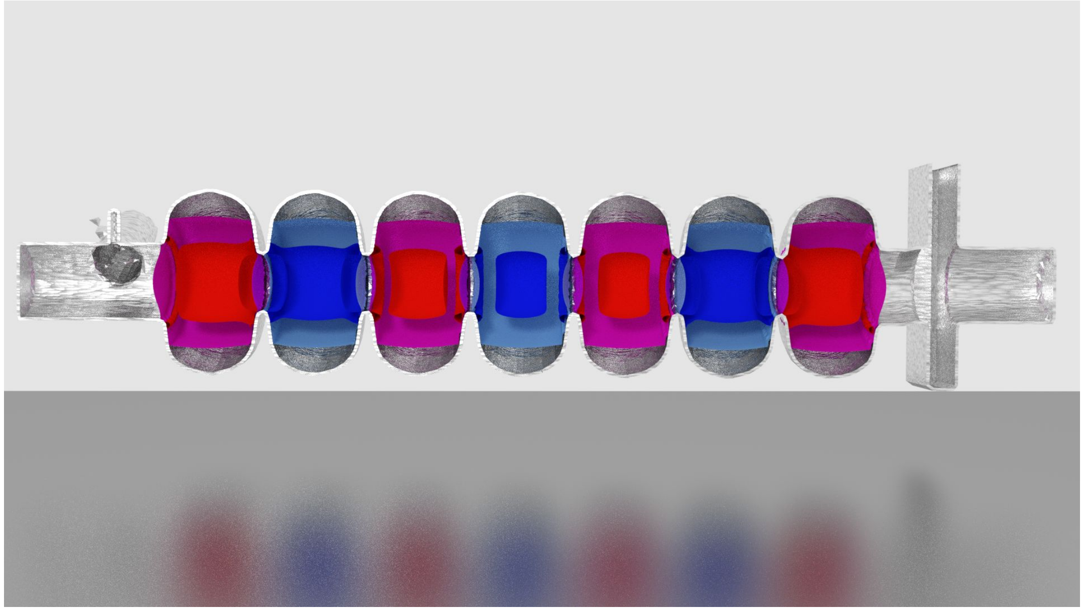
- We conduct research to benefit national labs and commercialize our simulation software - both industry and academic customers

- This project is synergistic and collaboratory with Jefferson Labs (JLAB) experimental efforts - Tom Powers

- At end of third year (NCE)

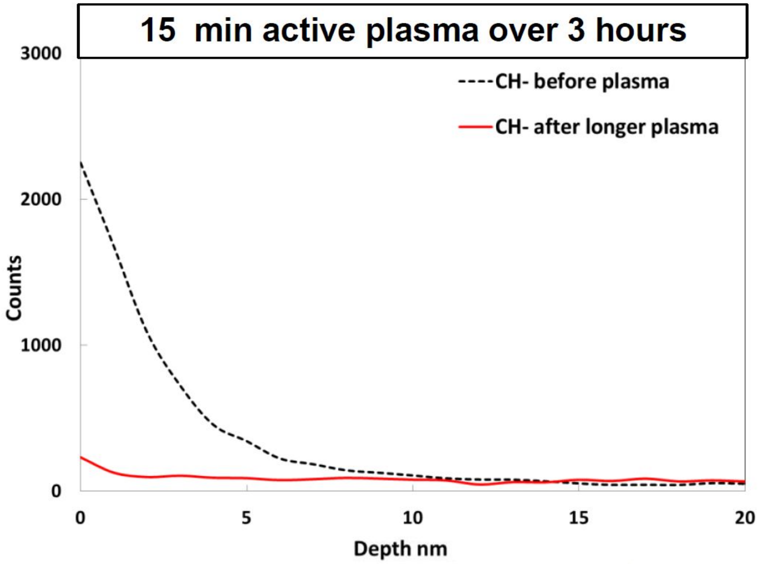
Overview

- Introduction to SRF cavities
- Overview of previous work
  - EM simulation
  - Ionization simulations
  - Hybrid model
  - Surface reactions
  - Simulations for JLAB
- Progress over the past year
  - Reaction diagnostics
  - More simulations for JLAB
- Other accomplishments



Introduction

- SRF cavities are used for particle acceleration
  - Acceleration gradients limited by surface impurities – cleaning required
- In-situ cleaning via plasmas is desired for limited downtime, cheap cleaning, etc.
- Desired simulation of this plasma because minimal diagnostics possible experimentally
- SBIR Phase I goal was proof-of-concept for plasma simulation allowing for Phase II to include more physics



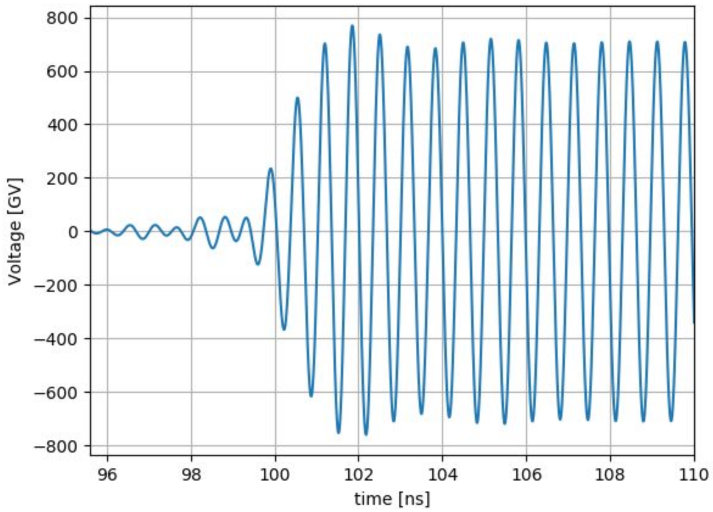
Project goals

- We want to understand:
  - How/where plasma forms
  - Transport of impurities freed from the surface
  - Questions that arise from JLABs experimental campaign

- What do we need to accomplish this?
  - Confirm EM accuracy in cavity geometry
  - Fundamental simulations of ionization
  - Development of surface reactions

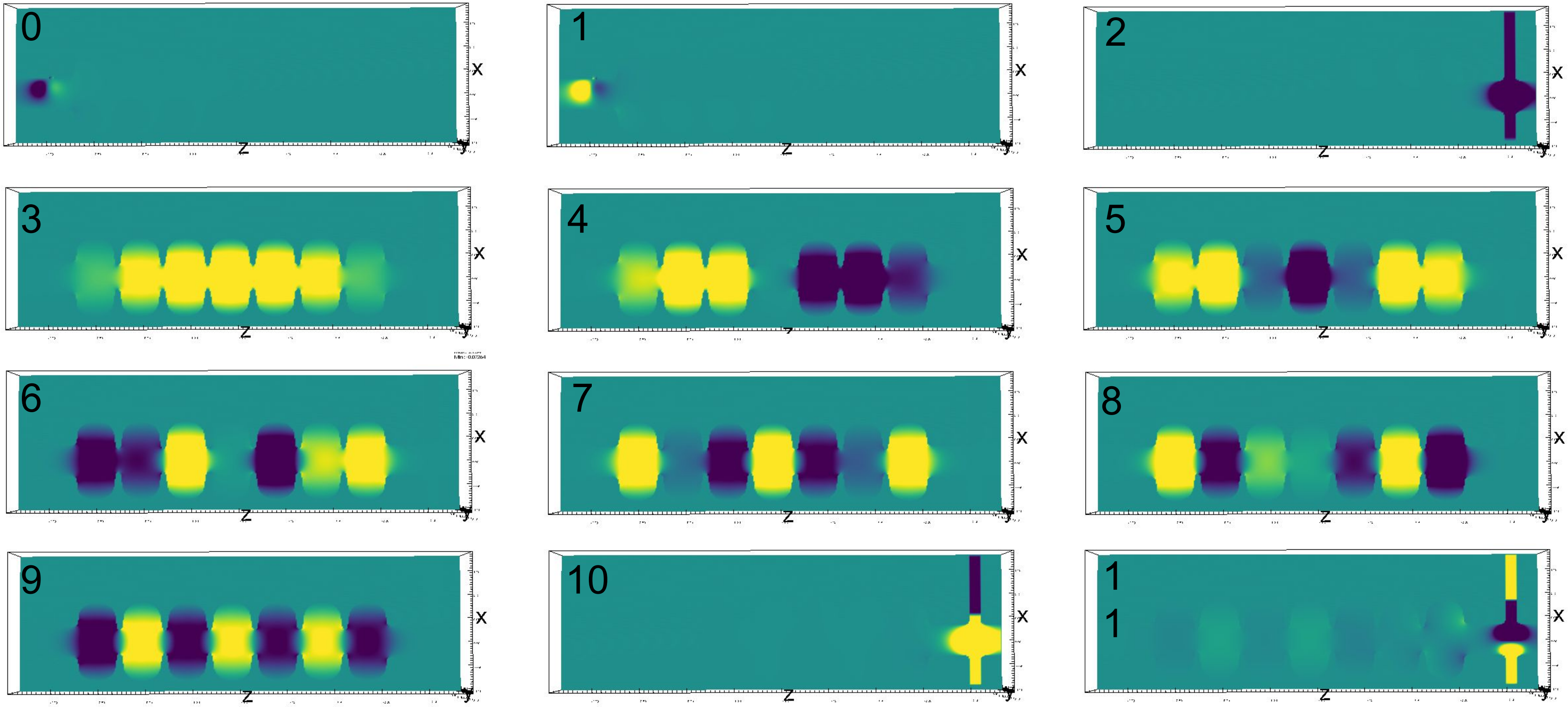
Electromagnetic simulation: Running

- Impose electric field of the modes we are trying to excite, in a band of frequencies
- Run long enough for the cavity to ring up (ie. in this case more than 100ns)
- After E-field source is gone, cavity will still continue to ring at the frequency of the resonant modes
- Simple analysis – Fourier transform resulting signal and look at peak frequency to find dominant mode
- But we can do better!



Electromagnetic simulation: Extract Modes

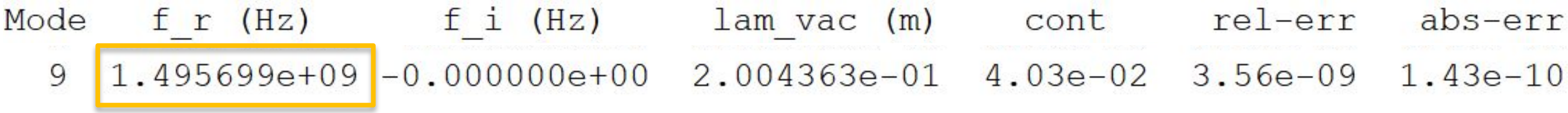
- Structures for all the found modes:



Extracting degenerate modes, Werner, 2008

Electromagnetic simulation: Pi-Mode

- Mode 9 is the pi-mode:



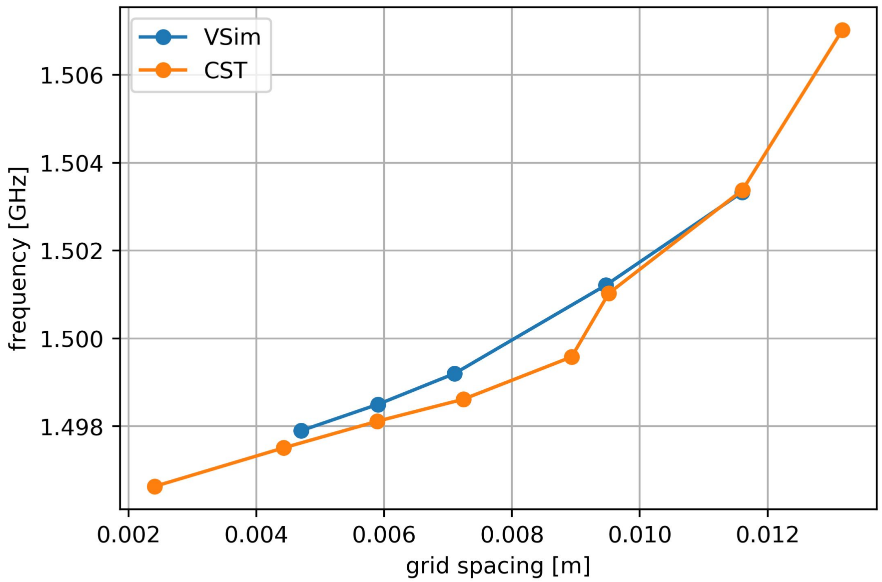
```
Mode     f_r (Hz)        f_i (Hz)        lam_vac (m)      cont        rel-err    abs-err
  9   1.495699e+09  -0.000000e+00   2.004363e-01   4.03e-02   3.56e-09   1.43e-10
```

- This frequency converges to the true frequency as dx→0, so the true frequency can be calculated via Richardson extrapolation

- The pi-mode frequency is:

  1.49549 GHz – VSim

  1.49561 GHz – CST



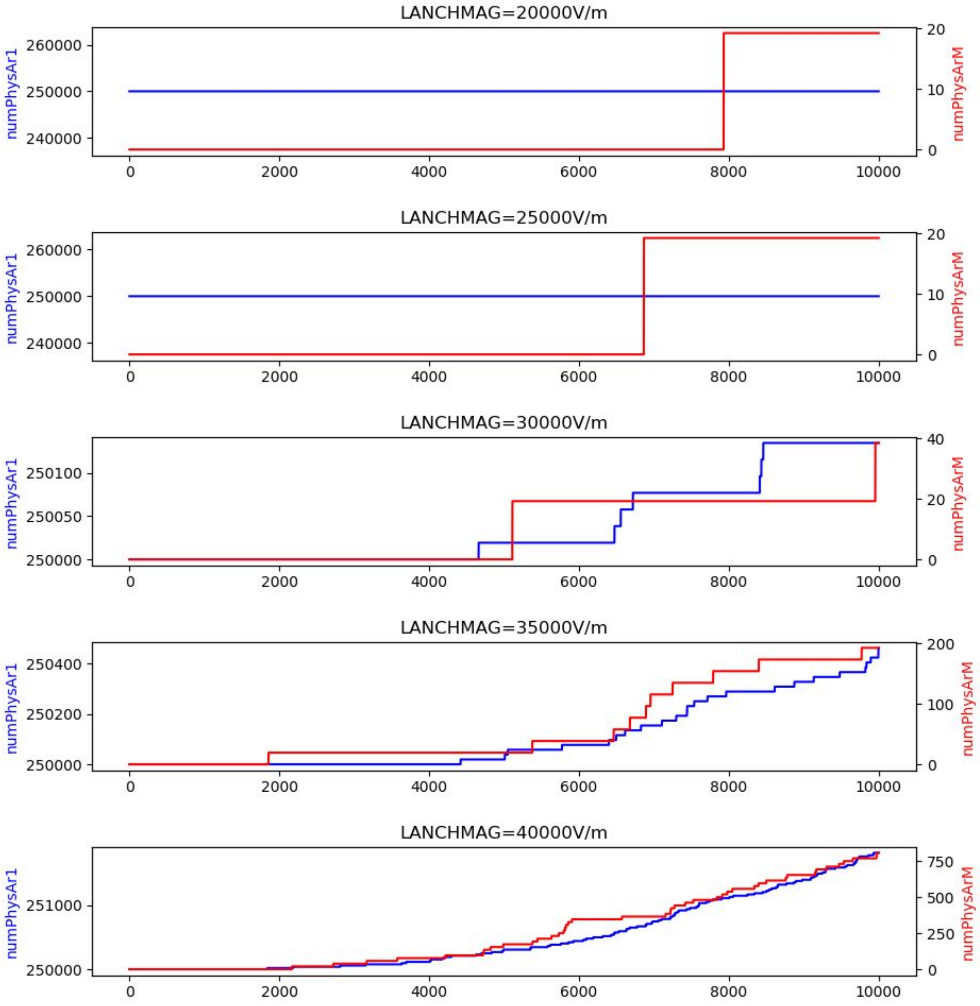
Plasma simulation: Introduction

- Electromagnetics have been validated, next step is plasma simulation

- Basic plasma formation process:
  - Free electrons accelerated by resonant EM modes
  - Impact ionization cascade is initiated, exponentially increasing the plasma density
  - Recombination and walls serve as sinks for plasma
  - Plasma density reaches equilibrium when source and sinks balance

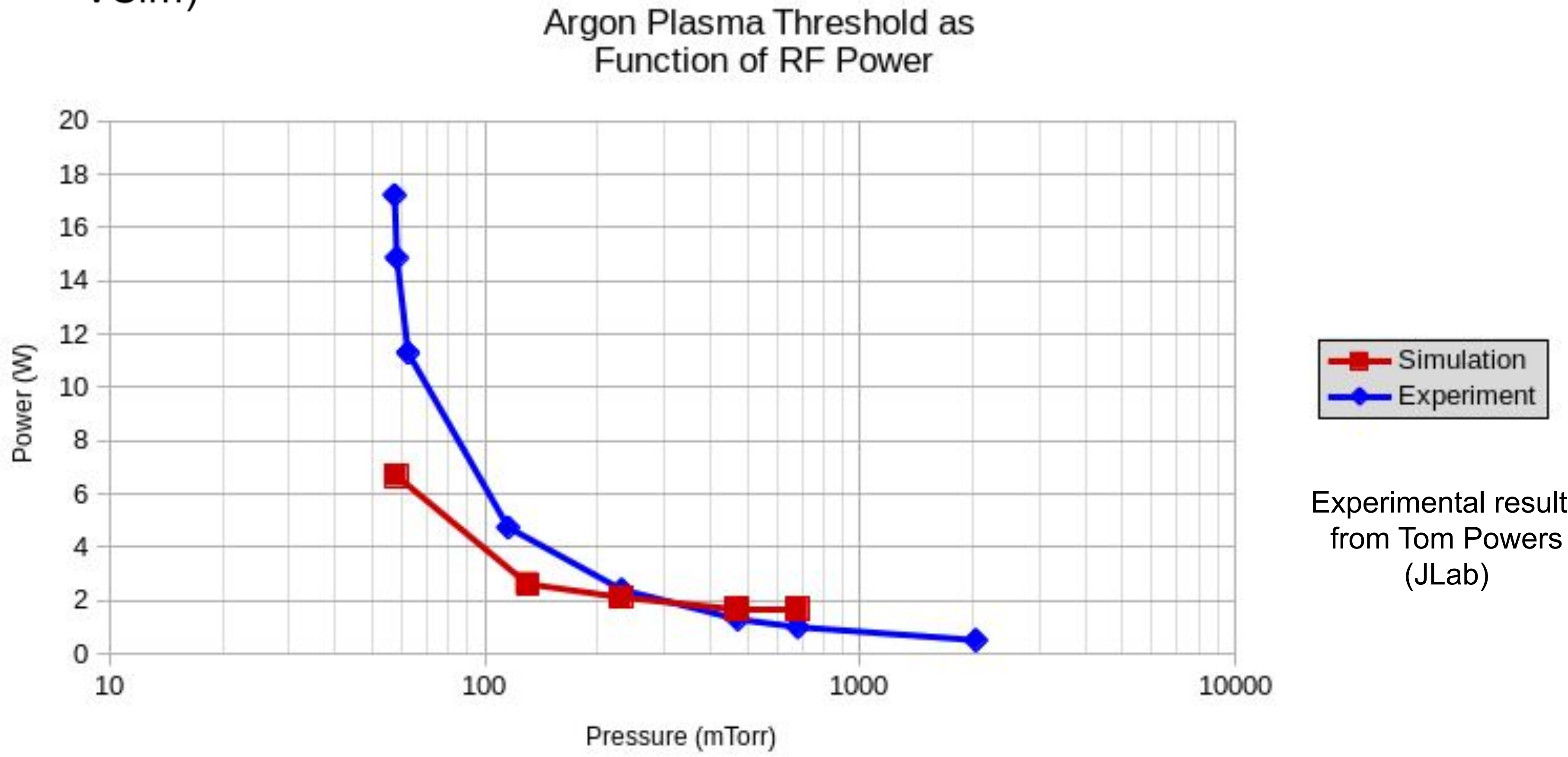
Plasma ignition simulation: Power Threshold Determination

- Multiple simulations each at different power
- Threshold is chosen to be where ionization cascade is seen to occur (ie. exponential growth in electron number)
- Reduce step size as we get closer to threshold (final resolution is 0.25W)



Plasma ignition simulation: Simulation vs. Experiment

- C100 cavity, $2\pi/7$ mode (1.91GHz) power threshold (periodic box simulated in VSim)



Experimental results from Tom Powers (JLab)

Hybrid Plasma Simulation

For full-device modelling, particle-in-cell simulation is expensive

Instead, implementing hybrid plasma model [Stanier 2018] where:

- electrons are represented as a fluid
- ions are modelled kinetically
- electric field is calculated via Ohm's Law

Allows us to step at electron bulk flow / sound speed time scales (instead of ω_{pe}) and relaxes requirement to resolve Debye length

$$\partial_t f_s + \boldsymbol{\nabla} \cdot (f_s \boldsymbol{v}) + (q_s/m_s)(\boldsymbol{E}^* + \boldsymbol{v} \times \boldsymbol{B}) \cdot \boldsymbol{\nabla}_v f_s = 0,$$

$$\partial_t \boldsymbol{B} = -\boldsymbol{\nabla} \times \boldsymbol{E},$$

$$\boldsymbol{E} = \boldsymbol{E}^* + \eta \boldsymbol{j} = -\boldsymbol{u}_i \times \boldsymbol{B} + \frac{\boldsymbol{j} \times \boldsymbol{B}}{ne} - \frac{\boldsymbol{\nabla} p_e}{ne} - \frac{\boldsymbol{\nabla} \cdot \overleftrightarrow{\Pi}_e}{ne} + \eta \boldsymbol{j},$$

$$(\gamma - 1)^{-1} [\partial_t p_e + \boldsymbol{\nabla} \cdot (\boldsymbol{u}_e p_e)] + p_e \boldsymbol{\nabla} \cdot \boldsymbol{u}_e = H_e - \boldsymbol{\nabla} \cdot \boldsymbol{q}_e,$$

Hybrid Plasma Simulation Benchmarks

- Developed the hybrid model implementation and conducted benchmarks to validate

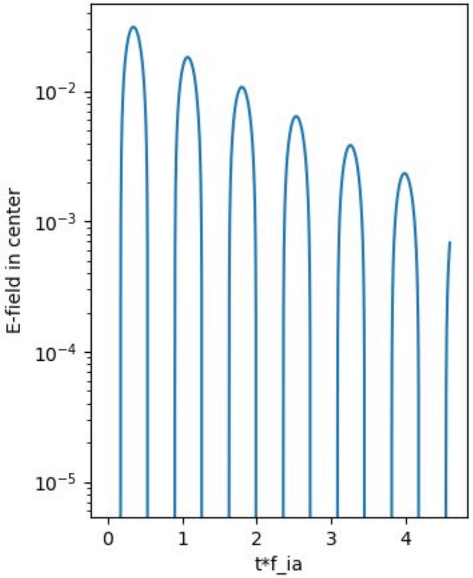
- Implemented boundary conditions for conductor so that cavity/shapes can be modelled

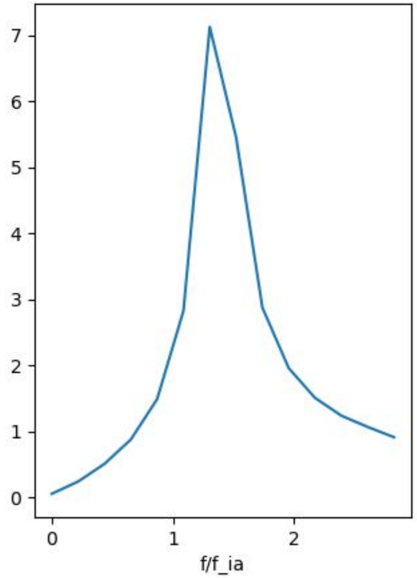
- We have chosen 2 physics problems, each of which will be simulated with full **fluids** (eg. MHD), **full kinetic** (PIC), and **hybrid**
  - Landau damping of ion acoustic wave: fluids should give wrong answer, hybrid and kinetic should give correct answer
  - GEM problem (reconnection): fluids can give close answer, depending on assumptions, hybrid and kinetic should both be correct

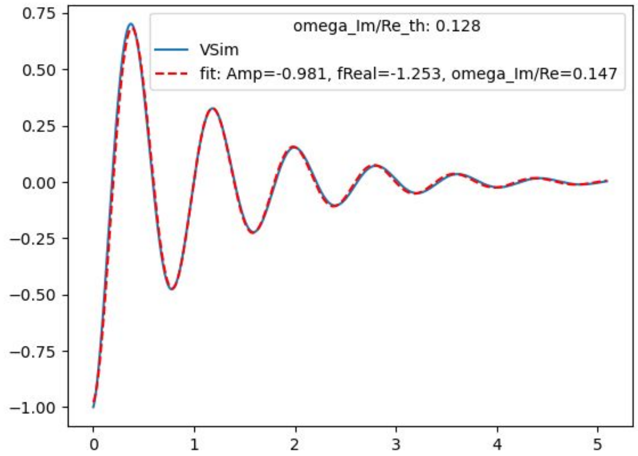
- In all cases speed should be fluids > hybrid > kinetic

Test #1: full kinetic model of Landau damping

- Landau damping is the exchange of energy between waves in cold ions and resonant hot electrons.
- Fully kinetic models of Landau damping are computationally expensive
- Hybrid models will capture the relevant physics and be computationally faster
- Damping rate and frequency match theory for ion acoustic Landau damping

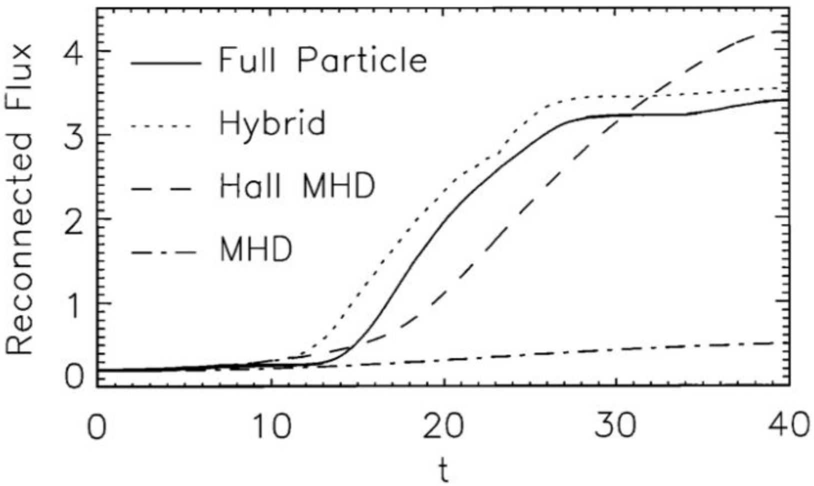




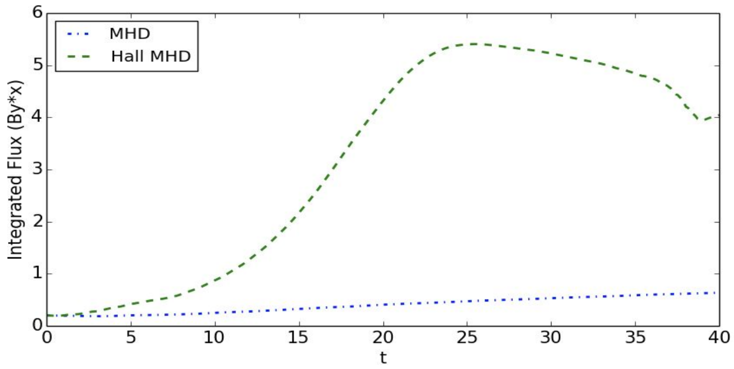


Test #2: extended MHD models of magnetic reconnection

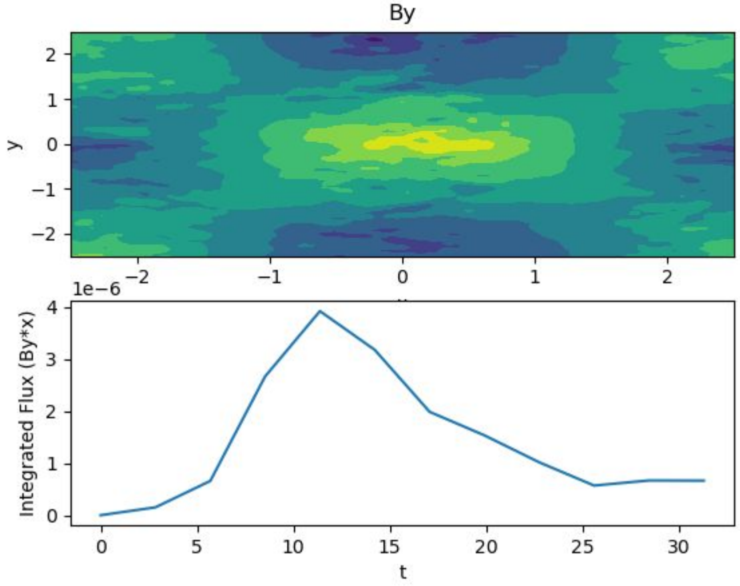
Birn '01



Our work



Fluid



Hybrid

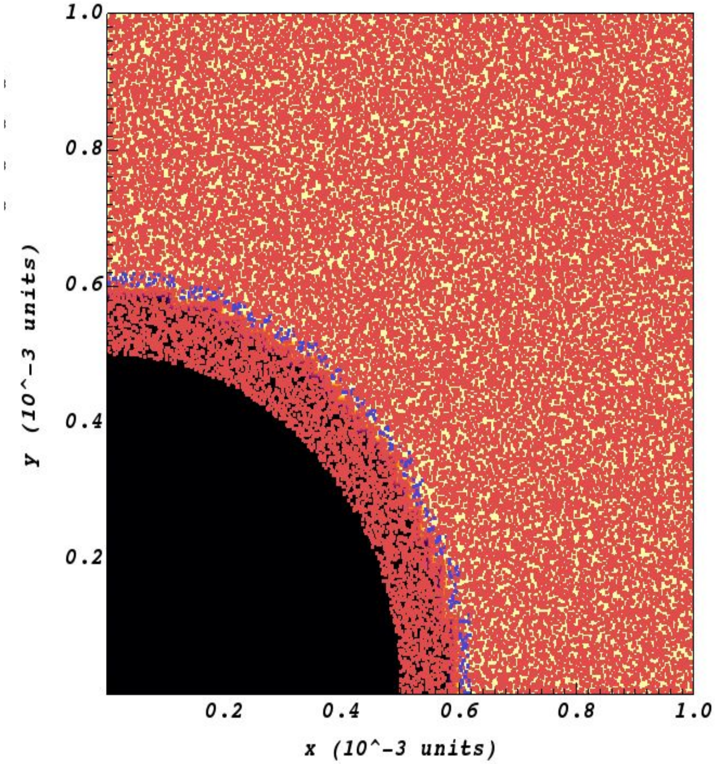
- We have reproduced several advanced fluid models of magnetic reconnection
- Hybrid model flux peaks to roughly correct value but drops back down - still investigating why

Surface reactions

- Existing framework within the software for bulk reactions - specify cross section and reactants/products

- Implemented ability to use boundary object as a reactant, thus limiting reaction location to boundary edges

- Now have the ability to react impurities on the cavity surface with the fluid and kinetic species within the plasma

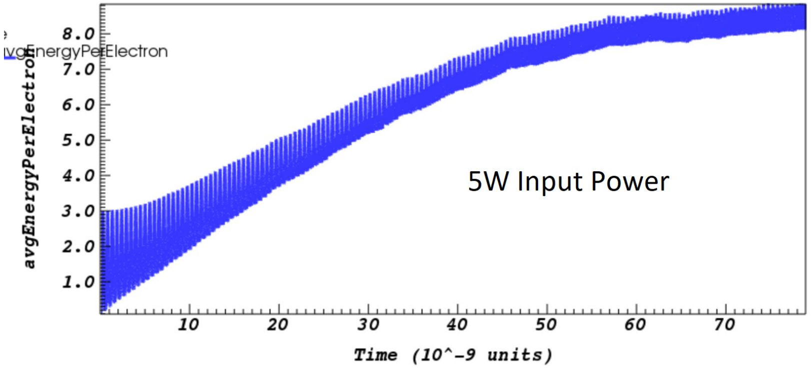


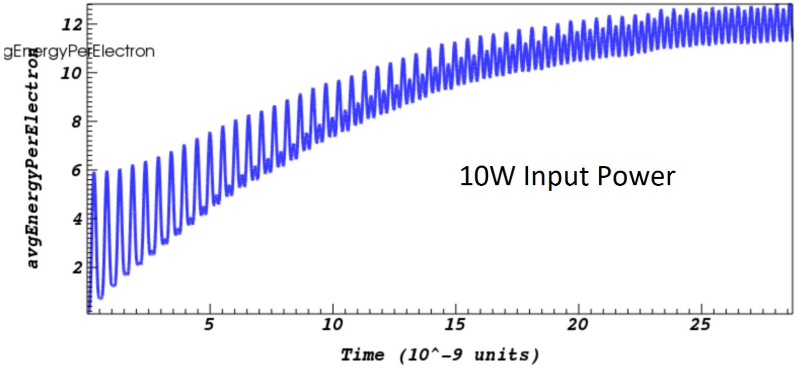
Experimentally Relevant Simulation for JLAB

- JLAB has an experimental campaign ongoing for plasma cleaning of cavities - we aim to be synergistic and supportive

- Of particular interest this past year was a simulation to determine the average energy of electrons ionized by an EM field of a particular power

- We were able to simulate these for a variety of powers and provide the results to JLAB





Additional Simulations for JLAB

- More simulation requests from JLAB led us to perform alternative simulations than those initially proposed

- Tom Powers wanted to know the expected steady state density of reactive Oxygen species for various values of input power and oxygen content in the gas mixture:
  - 1%, 8%, 20% oxygen (argon being the other gas)
  - 5W and 10W of input power

- For each combination we cannot run just a single simulation, but need to first run a kinetic simulation followed by a fluid simulation

Additional Simulations for JLAB

Kinetic simulation:

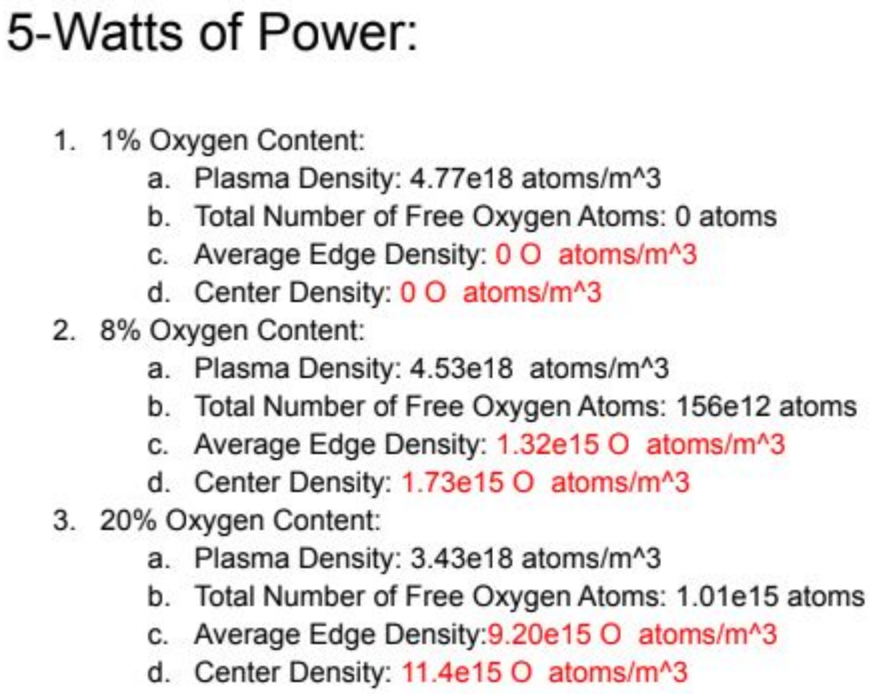
- Using similar technique to the ionization cascade simulations, we use kinetic simulation to determine the ionization/dissociation rates for Oxygen in a given gas mixture
- The rate is a function of the energy of the electrons/ions, which is a function of the electric field value

Fluid Simulation:

- The reactive oxygen density at the surface is important for impurity removal
- Fluid simulation estimates the equilibrium profile at longer time scales over many RF periods - main source is in the center of the cavity cells while the edge is a sink

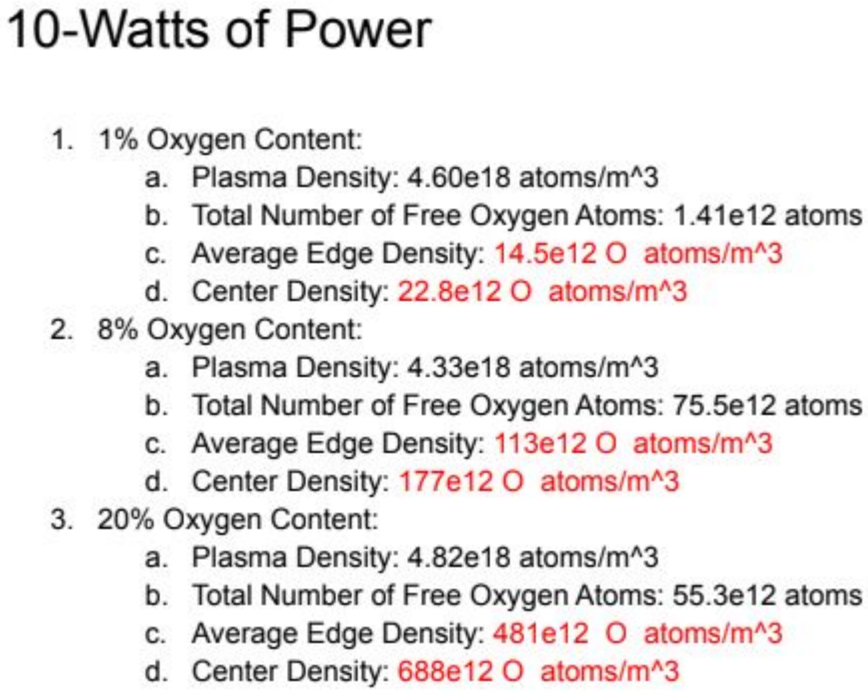
Additional Simulations for JLAB

Results:



5-Watts of Power:

1. 1% Oxygen Content:
    a. Plasma Density: 4.77e18 atoms/m^3
    b. Total Number of Free Oxygen Atoms: 0 atoms
    c. Average Edge Density: 0 O atoms/m^3
    d. Center Density: 0 O atoms/m^3
2. 8% Oxygen Content:
    a. Plasma Density: 4.53e18 atoms/m^3
    b. Total Number of Free Oxygen Atoms: 156e12 atoms
    c. Average Edge Density: 1.32e15 O atoms/m^3
    d. Center Density: 1.73e15 O atoms/m^3
3. 20% Oxygen Content:
    a. Plasma Density: 3.43e18 atoms/m^3
    b. Total Number of Free Oxygen Atoms: 1.01e15 atoms
    c. Average Edge Density:9.20e15 O atoms/m^3
    d. Center Density: 11.4e15 O atoms/m^3

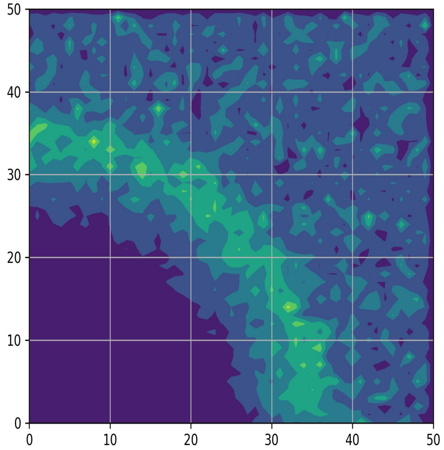


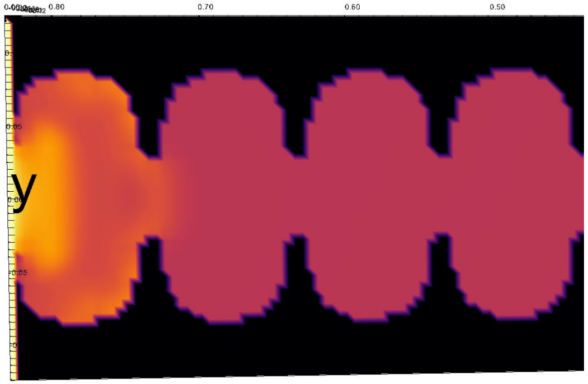
10-Watts of Power

1. 1% Oxygen Content:
    a. Plasma Density: 4.60e18 atoms/m^3
    b. Total Number of Free Oxygen Atoms: 1.41e12 atoms
    c. Average Edge Density: 14.5e12 O atoms/m^3
    d. Center Density: 22.8e12 O atoms/m^3
2. 8% Oxygen Content:
    a. Plasma Density: 4.33e18 atoms/m^3
    b. Total Number of Free Oxygen Atoms: 75.5e12 atoms
    c. Average Edge Density: 113e12 O atoms/m^3
    d. Center Density: 177e12 O atoms/m^3
3. 20% Oxygen Content:
    a. Plasma Density: 4.82e18 atoms/m^3
    b. Total Number of Free Oxygen Atoms: 55.3e12 atoms
    c. Average Edge Density: 481e12 O atoms/m^3
    d. Center Density: 688e12 O atoms/m^3

Other accomplishments

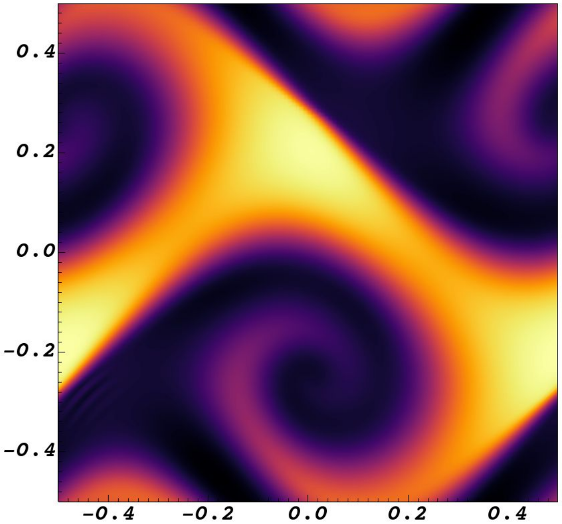
- We have highlighted the major work we've been doing, but the project consisted of a variety of other tasks that we've made progress on:
    - Reaction statistics recording (collision frequency as a function of space)
    - GUI improvements allowing alteration of CAD geometries *in situ*
    - Euler fluid implementation on CPU/GPU with conformal boundaries (neutral fluid)
    - Market research and analysis of potential customers

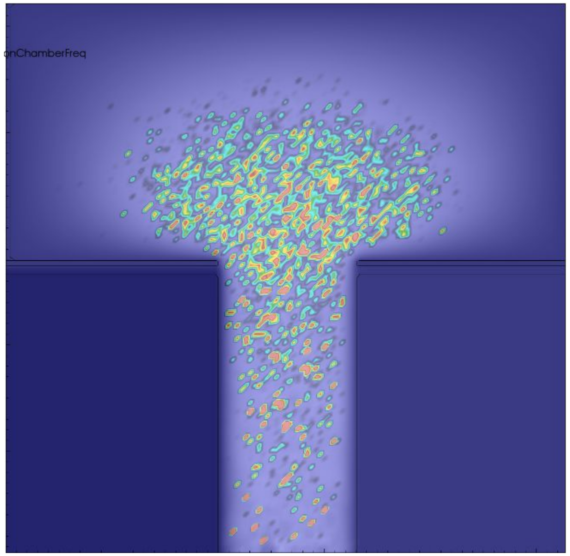


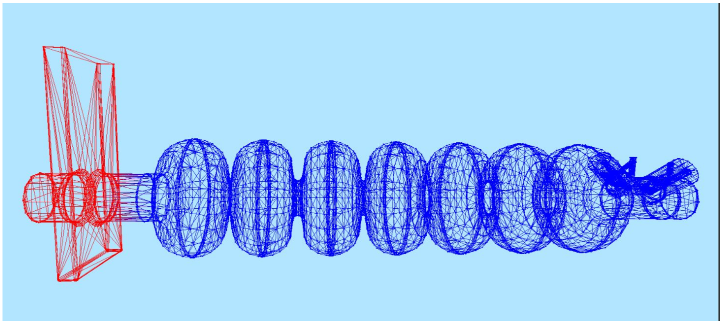


Project Outlook

- Developed features will be released in VSim12 in September 2022:
    - Euler fluid model
    - Hybrid fluid model
    - Reaction diagnostics
    - CAD manipulation







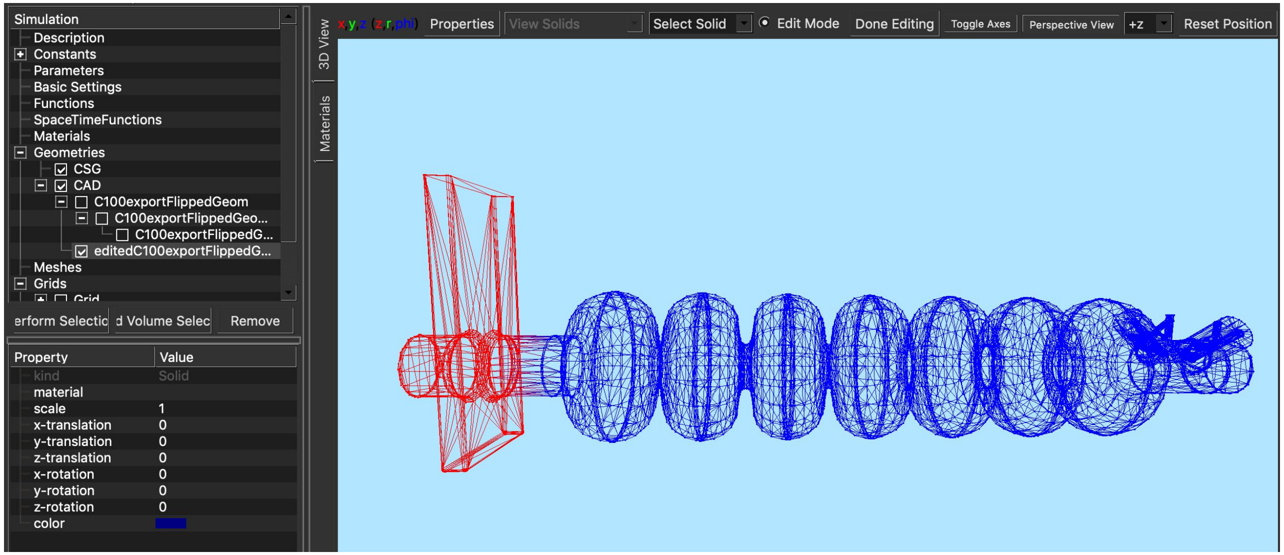
Thank you!

Questions?

Funding through grant
SBIR DOE-FOA-0001770

Other accomplishments

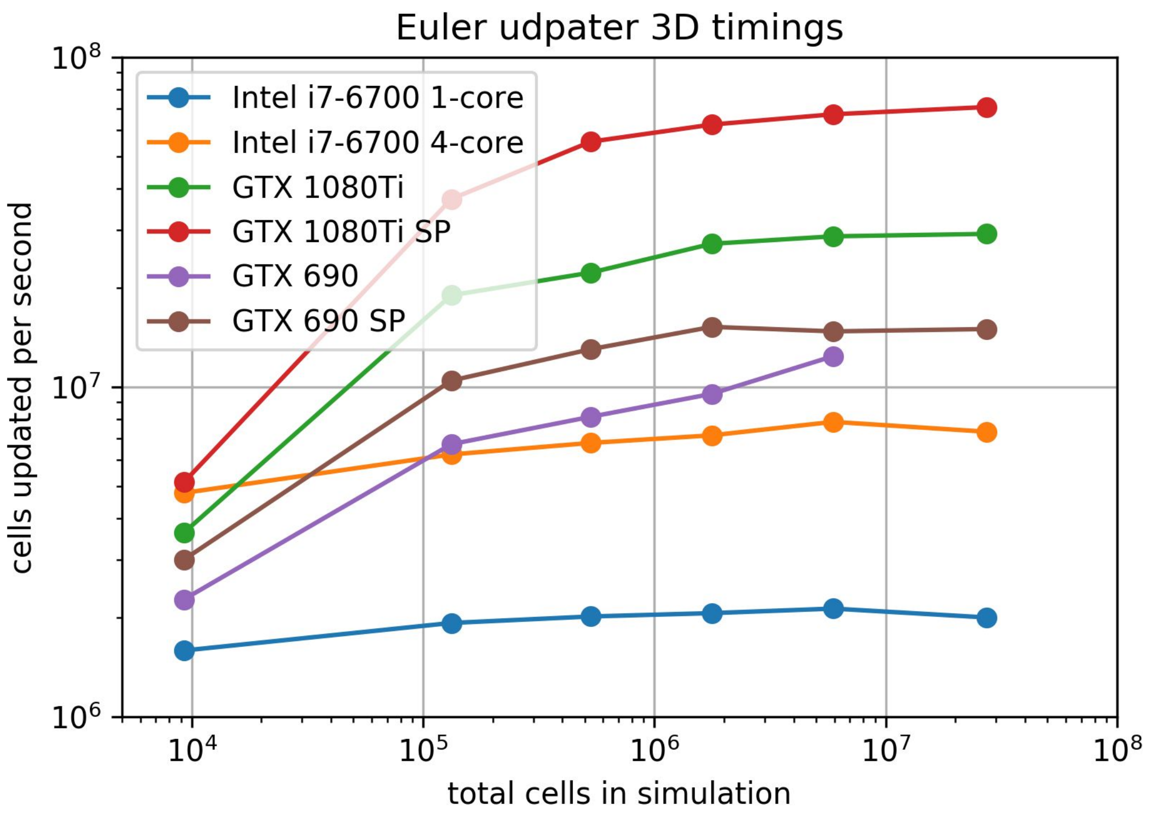
- We have highlighted the most interesting physics work we've been doing, but the project consisted of a variety of other tasks that we've made progress on:
  - **GUI improvements allowing alteration of CAD geometries *in situ***



Property	Value
kind	Solid
material	
scale	1
x-translation	0
y-translation	0
z-translation	0
x-rotation	0
y-rotation	0
z-rotation	0
color	🟦

Euler fluid timings

We see considerable speedup using GPUs for our fluid solve



Plasma ignition simulation: Assumptions

- Cavity is large (1m long) with 3D geometry means grid is too big for quick simulation because we must resolve Debye length (~1e-5m) and mean free path
- Let's assume the following:
  - Walls do not play a large role in initial ionization cascade
  - Set of important reactions includes direct ionization, multi-step (metastable) ionization, recombination, inelastic scattering
  - Ionization cascade will result in exponential increase in ions/electrons
- Simulation is periodic box with homogenous E-field oscillating at f=1.91GHz for the 2pi/7 mode (compare with experiment)

Plasma ignition simulation: Converting from E to P

- In simulation we control electric field, *E*, but need to compare to experimental value of input power, *P*
- Steps:
    - Equation: $P = \frac{f_0 U}{Q} = \frac{f_0 \epsilon_0 \langle E \rangle^2 V}{2Q}$
    - Power conversion requires *Q* of cavity. Use data from Tom Powers (*Q* = 931 for $2\pi/7$ mode)
    - Run EM simulation of SRF cavity to get ratio of E_{max} to average field, $\langle E \rangle$, because E_{max} is where ionization will occur (17.2 ×)