Integrated Multiple Effects Software for Nuclear Physics Applications

David Smithe (PI, Presenter)
Peter Stoltz, Robert Crockett
Tech-X Corporation, Boulder, CO, USA 80303

Haipeng Wang, Gary Cheng
Thomas Jefferson National Accelerator Facility
Newport News, VA, USA 23606

Grant #: DE-FG02-08ER85184

Company overview

- Tech-X: A software and R&D corporation with more than 60 employees, roughly 2/3 PhDs
- Several offices in U. S.
  - Headquarters in Boulder, Colorado
- Office in U.K.
- Resellers in Korea, Taiwan

Abstract

Nuclear physics accelerators are powered by microwaves which must travel in waveguides between room-temperature sources and the cryogenic accelerator structures. The ohmic heat load from the microwaves affects the cryogenic thermal conduction problem, via the temperature-dependant surface resistance and thermal conductivity. Integrated EM & thermal analysis of this difficult non-linear problem is being done with the VORPAL finite-difference time-domain simulation tool.

We overview tool capabilities, thermal benchmarking work with a complex HOM feed-through geometry, and ongoing EM & thermal design work, done in collaboration with researchers at the Thomas Jefferson National Accelerator Laboratory.

This work is part of an effort to generalize the VORPAL framework to include generalized PDE capabilities, for wider multi-physics capabilities in the accelerator, vacuum electronics, plasma processing and fusion R&D fields, and we will also briefly overview these commercial and other applications of the emerging technology.

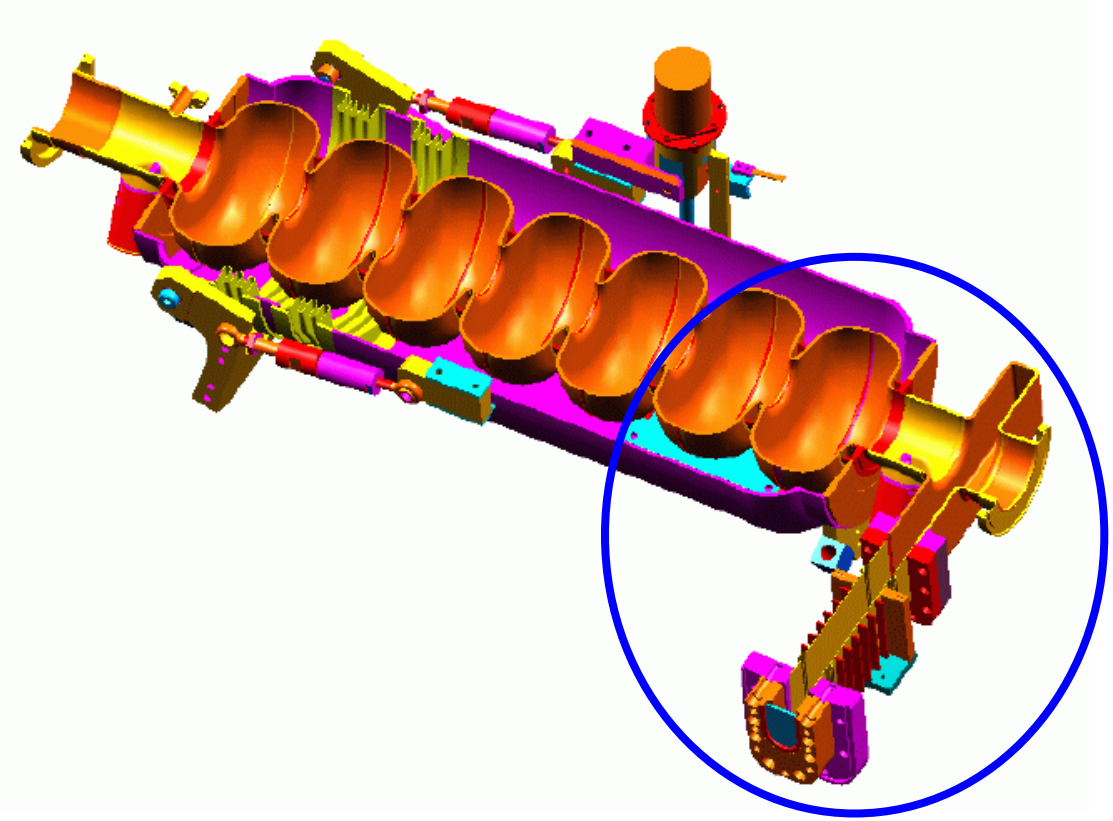
What is "Integrated Multiple Effects"?

- Many modeling tools solve a specific problem that they are good at, and then the user struggles to merge that data with other tools, which might typically have different:
  - Physics assumptions and simplifications
  - Data format and representation
  - Computational platform issues

- But ***multiple effects*** problems require coupling solvers from very different areas of physics (e.g., for accelerators)
  - Electromagnetic & Thermal (HOM couplers - staying cryogenic)
  - Thermal & Mechanical (Cavity expansion - re-tuning)
  - Thermal & Magnetic (Shielding of Earth's Magnetic-field)
  - Plasma & Thermal (Multipactor - staying cryogenic)

Problem of interest: superconducting RF cavities, input and HOM couplers

- Ohmic wall heating is a problem that combines EM and Thermal, and is the focus of most of our activity.
- Input waveguides and High-Order-Mode couplers connect cryogenic parts to normal conducting parts.
- Important for all cryogenic accelerators (FRIB, etc.)



From “Design and construction of the prototype cryomodule renascence for the cebaf 12 gev upgrade,” C. E. Reece, G. Ciovati, I. E. Campisi, E. F. Daly, J. Henry, W. R. Hicks, J. Hogan, P. Kneisel, D. Machie, J. Preble, T. Rothgeb, J. Sekutowicz, K. Smith, T. Whitlatch, K. M. Wilson, M. Wiseman, and G. Wu, Jefferson Lab, Newport News, VA 23606, USA.

VORPAL is the name of our multi-physics software

- There are now several Multiple Effects Software tools in the commercial market. We compete, and we are also unique.

- Tech-X's VORPAL software has several unique capabilities
  - Familiar with NP accelerator science and research
    - Used in DOE Scientific Discovery (SciDAC) programs.

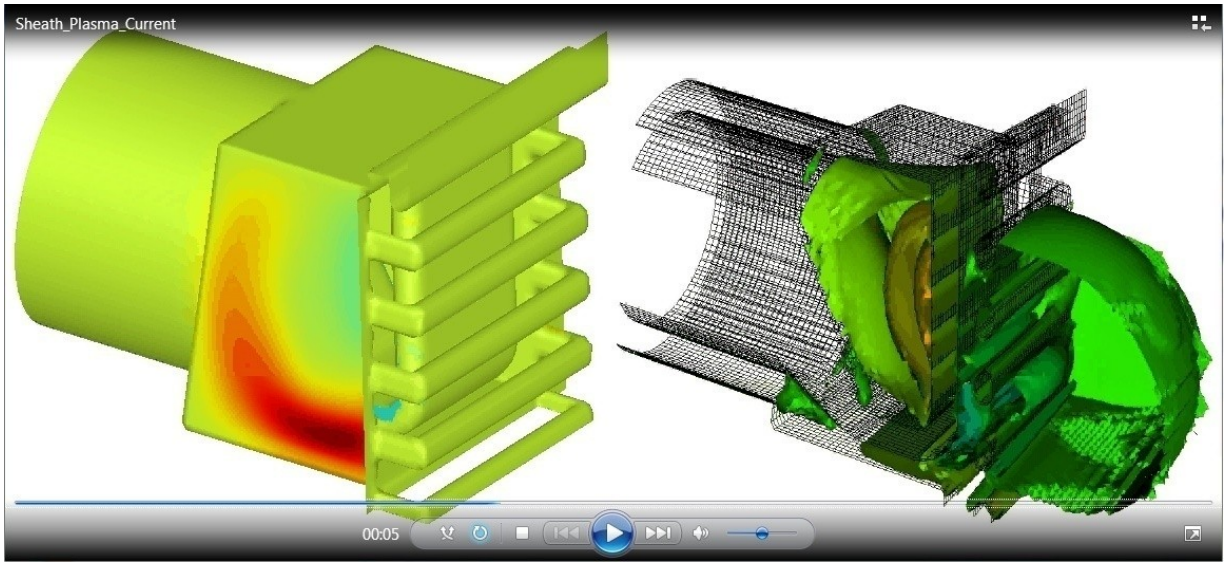
    "All DOE collaborators get to use tools for free, at the DOE computational facilities."
  - Capability to do particles, including self-consistent non-linear dynamics
  - Strong emphasis on Cross-platform (Windows, Apple, Linux, NERSC)
  - Designed for parallel (MPI) from the beginning

- And VORPAL is also now a leader in using GPU computing to give order of magnitude speedup *(earlier talk by Paul Mullowney)*
  - Fields on GPU are impressive
  - Particles are in progress

Improved user interface and communications for better commercial competitiveness

- A primary corporate goal the past year has been the development of a more advanced Graphical User Interface, called Composer, with integrated Visit graphics.

- We have initiated a series of IEEE webinars
  - Vacuum Electronics (Oct 27)
  - Plasma Processing DBD (Dec 1) *(already 81 signed up for this)*

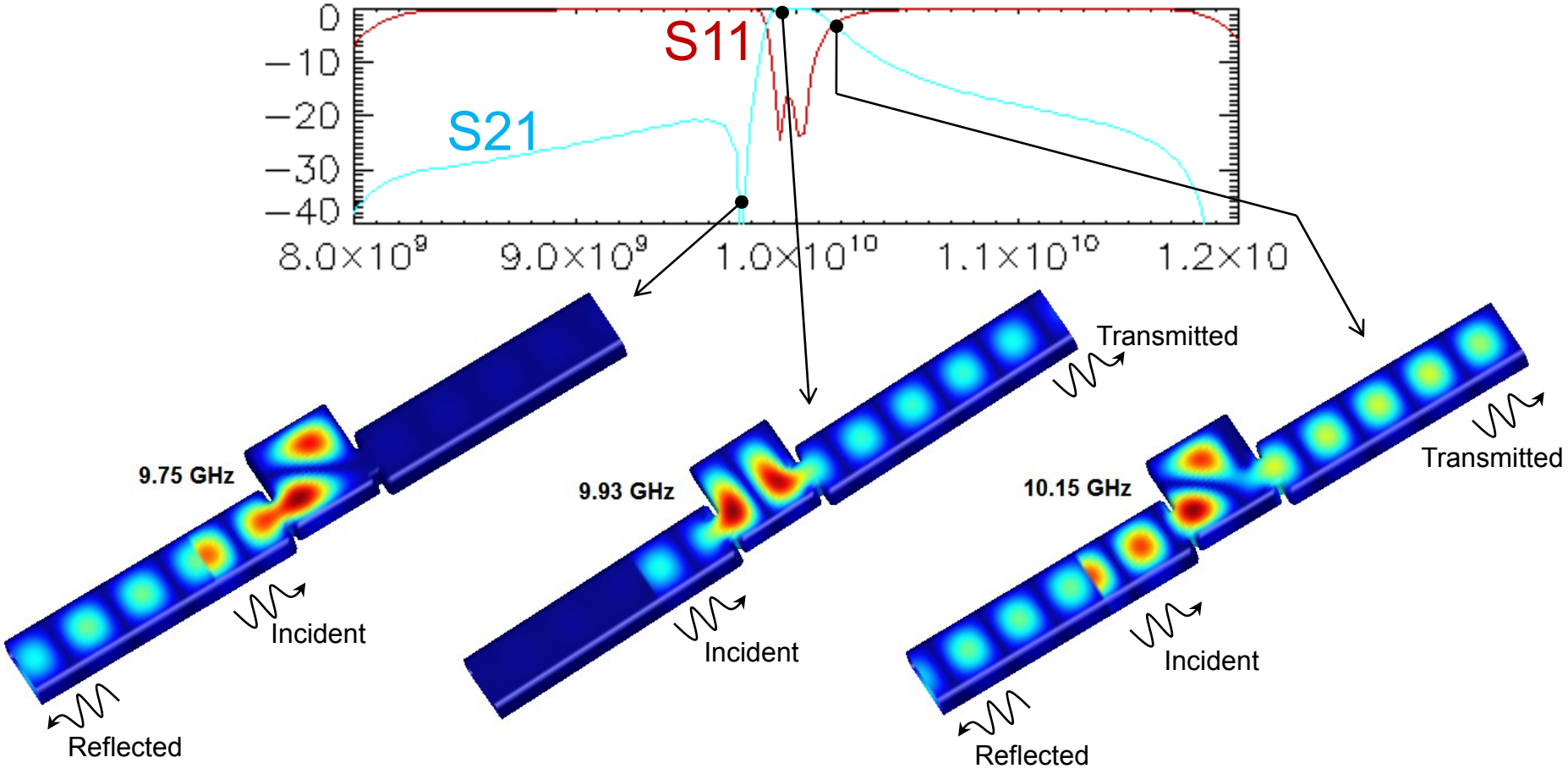


Multiphysics Simulation
- E&M
- plasma
- sheath

- Visit graphics

Improved example database for easier commercial applications

- Examples and macros for specific devices and analyses
  - Mode Analysis, sMatrix *(below)*, Wave Scattering, Thermal Analysis
  - LPA, multipacting, Gas Stopping, Two Stream, etc.



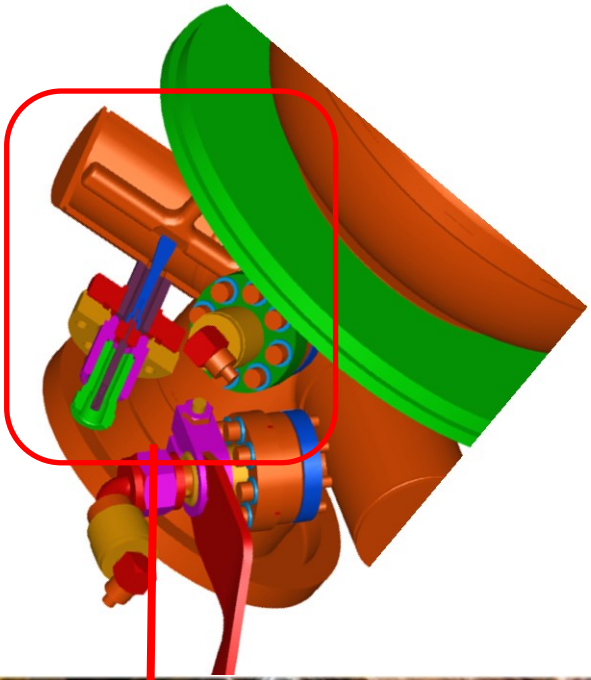
Major Accomplishments of the Phase II project

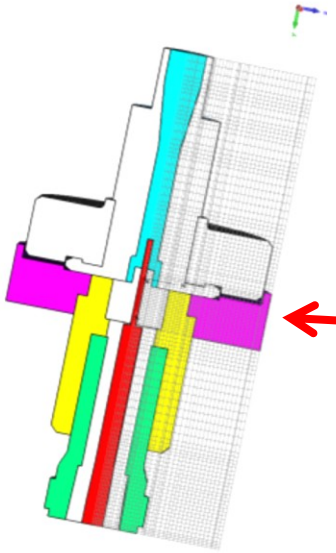
- Developed “cut-cell” finite-volumes thermal treatment for complex geometries, consistent with E&M modeling
- Benchmarked a cryogenic problem (HOM feed-through) against measurement and other software, in collaboration with JLab
- Ongoing work:
  - E&M + Thermal design work to evaluate crab cavity thermal loading
  - Implicit solver work, for transient modeling of quench-type event
- This project is a primary engine driving the emerging multi-physics capability of the commercial VORPAL software

Year 1 benchmarking case

Benchmark is the HOM coaxial coupler feed-through, for which prior, and on-going, analysis exists, and for which laboratory measurement data exists.

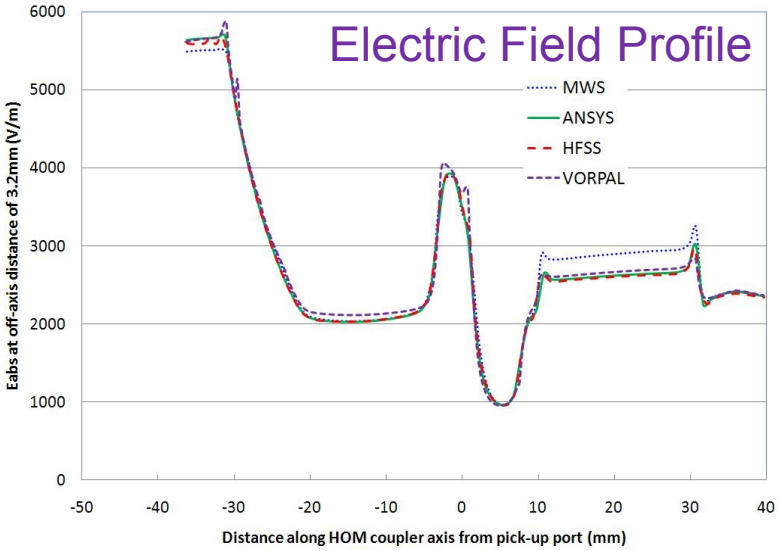
(G. Wu, H. Wang, R. Rimmer, and C. Reece, "Electromagnetic simulations of Coaxial Type HOM Couplers," JLAB-ACC-05-418, also THP58 in Proceedings of 12th SRF Workshop, Cornell University, July 2005.)

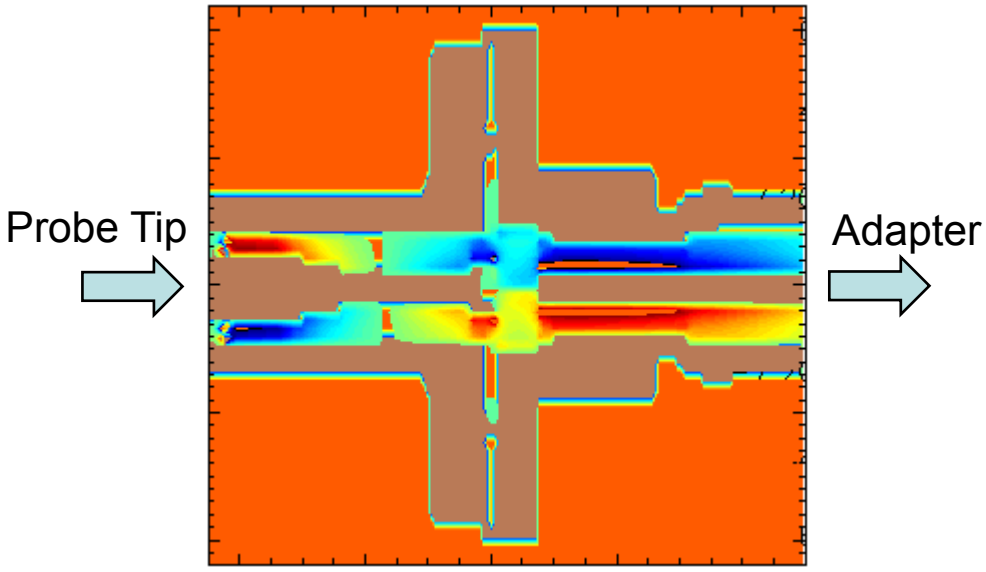


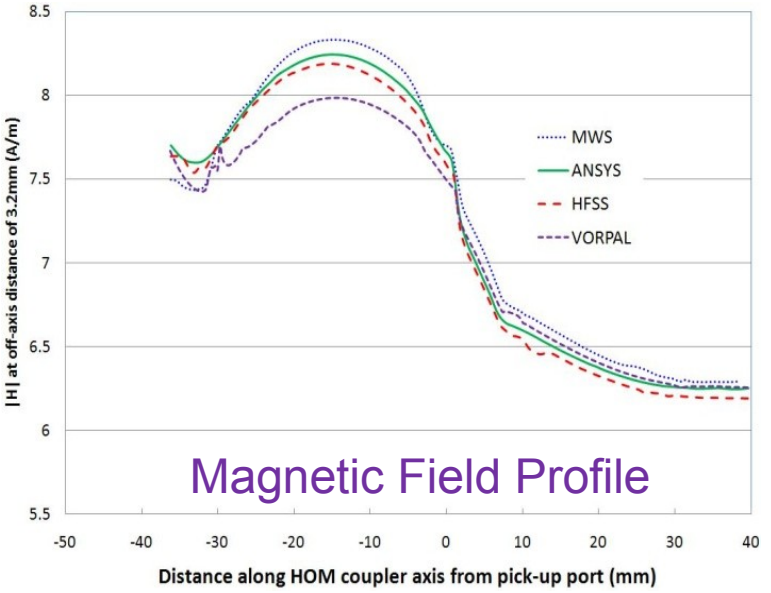


Benchmark results in good agreement with other codes and measurements

- The outer coaxial probe tip of the coupler is extended to form a coaxial line.
- 1 watt power is fed into probe end.
- Electric and magnetic profiles, S11, and S21, from MWS, ANSYS, HFSS, and Vorpal are compared.
- Excellent E field, B field more sensitive to grid resolution.



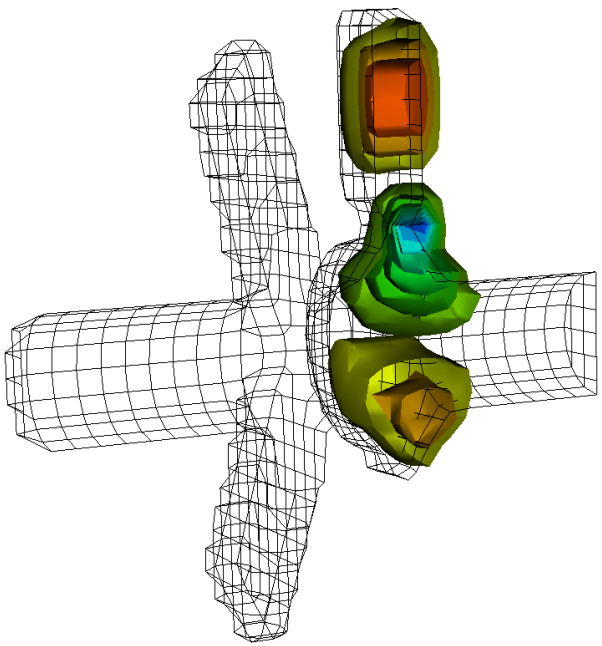


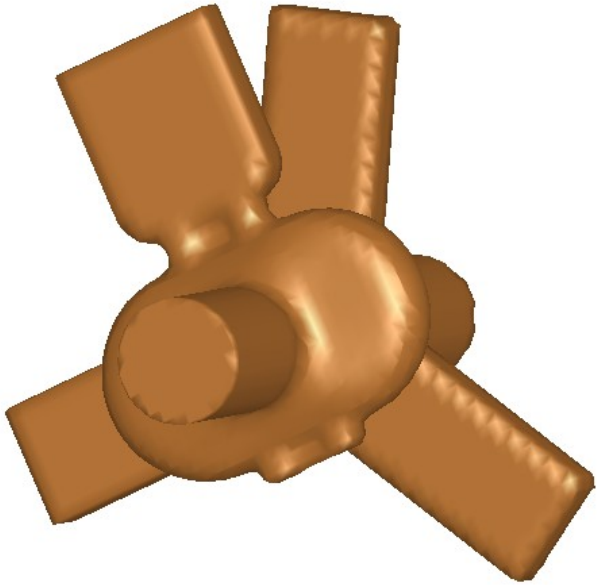


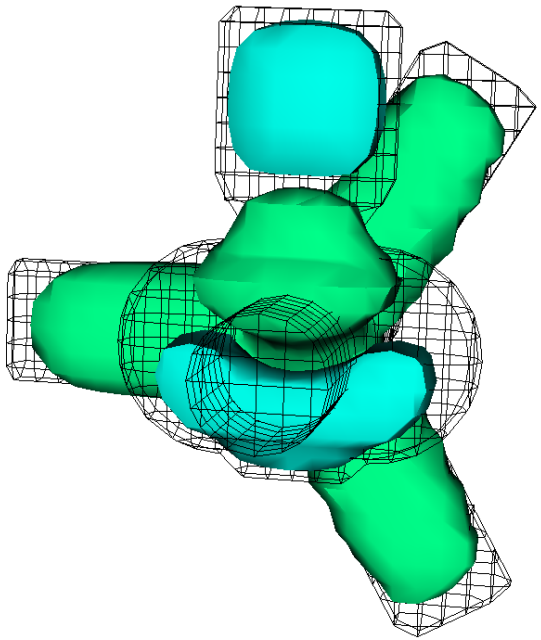
Year 2 design work is just underway

- Crab cavity thermal analysis is needed (no measurements at this point)

- First goal is to estimate the thermal load from the operating mode, into waveguides, and to determine an optimum heat station configuration for the waveguides.







Additional work in progress – transient analysis

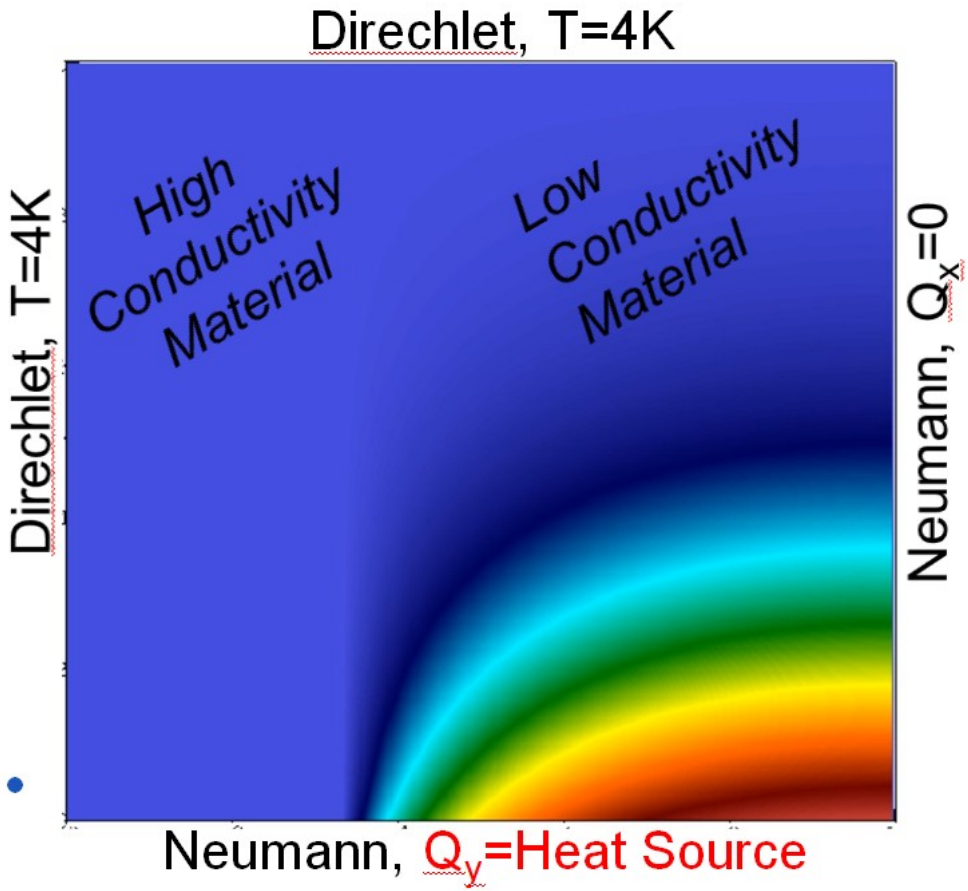
- The benchmarking and design work focused on steady-state problems:
  - Equation: $\nabla \cdot k(T) \nabla T = 0$, *and b.c.'s*
  - This can be done with a iterative solve, or with a matrix inversion.

- A problem of interest is the quench transient, which requires solving the time-dependent heat equation:
  - Equation: $C(T)\, \partial_t T = \nabla \cdot k(T) \nabla T$, *and b.c.'s*
  - This requires a true backward euler step, and matrix inversion.

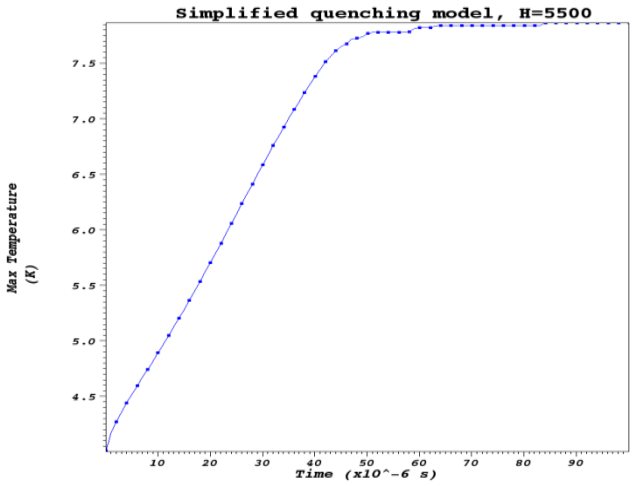
- We use the Trillinos library for our solver
  - Employed a summer intern from CU to set up the solve, determine best selection of options, preconditioners, etc.
  - Verified practical operation in situations of interest
    - strong *k(T)* behavior, adjoining materials with 10^4 difference in *k(T)*.

Transient analysis test case – "hot spot" figure of merit

- Rectangular domain, two materials, combination of Direchlet and Neumann boundaries at domain edges.



Max temperature vs. time



- In progress, boundaries for complex geometry

Program Status

- In Extended year. 50% of Year 2 task → Extended Year.
- Task 4 is the primary focus for the remaining time, with some additional focus on Task 8, Advanced Algorithms.
- Presently 4 people active on the project (2 at Tech-X and 2 at JLab). Entire project will have involved at least 8 personnel.

Original Schedule

	QUARTERS DURING PROJECT							
TASK	1	2	3	4	5	6	7	8
Task 1. Cut-cell Volume Capability	1	¾						
Task 2. Cut-cell Surface Capability		½	¾	½				
Task 3. Thermal Benchmarking	½	½	½	½				
Task 4. Application to Thermal Design					½	½	½	½
Task 5. Geometry Primitives				½	½	¼	½	
Task 6. Materials Table		¼			½	½		
Task 7. Advanced Materials and BC's				½		¾		½
Task 8. Advanced Algorithms	½		¼		½		½	
Task 9. Additional Multiphysics							½	1

Conference presentations

- Invited Talk: "Integrated EM & Thermal Simulations with upgraded Vorpal Software," D. Smithe, Peter Stoltz, Dan Karipides, H. Wang, G. Cheng, Newport News, VA (PAC 2011).

- "Multi-Physics Simulations with VORPAL," David Smithe, Peter Stoltz, Ming-Chieh Lin, Dan Karipides, Haipeng Wang, Kai Tian, Gary Cheng, 37th IEEE Conference on Plasma Science, Norfolk, VA (ICOPS 2010).

- "Multi-Physics Simulations with VORPAL," David Smithe, Peter Stoltz, Ming-Chieh Lin, Daniel Karipides, Haipeng Wang, Gary Cheng, Kai Tian, 2010 International Vacuum Electronics Conference, Monterrey, CA (IVEC 2010).

Looking towards the future: many other multi-physics areas

- Expect more work for particle / plasma thermal couplings. (e.g., Multi-pactor, affects DOE NP accelerators, also important in general to all vacuum electronics)
- Surface and plasma chemistry for plasma processing community
- Fluid flow (convection) (suggested by Jlab, others)
- Stress / strain, thermal stress (suggested by JLab)
- Magnetic shielding (suggested by JLab)

Quick Summary

- Project is extended one year, with expectation of finishing original proposed task plan
- JLab CRADA collaboration moving from benchmarking to design modeling
- Good benefit for EM & Thermal modeling of Nuclear Physics accelerator components
- Good commercialization effort, activity, and interest