Integrated Multiple Effects Software for Nuclear Physics Applications

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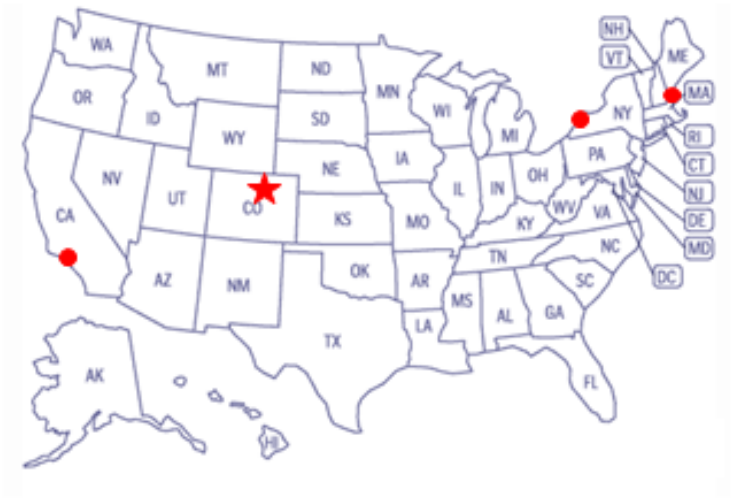
Company overview

- Tech-X: A software and R&D corporation with more than 60 employees, roughly 2/ 3 PhDs
- Offices in U. S. and Europe
  - Headquarters in Boulder, Colorado
- Resellers in South Korea, India, and Taiwan and China.
- More detail in talk by D. Bruhwiler.



Abstract

Nuclear physics accelerators are powered by microwaves which must travel in waveguides between room-temperature sources and the near-absolute-zero temperature of the accelerator structures. Tech-X has been developing multiple effects software (called VORPAL), which is designed for modern parallel computing platforms.

VORPAL is already a leading and sophisticated microwave simulation tool, and this SBIR project adds a more general multi-physics framework to VORPAL, with project focus on combined EM & thermal analysis.

We report on the first year task work of the project, highlighting the thermal benchmarking work done on a complex HOM feedthrough geometry, done in collaboration with researchers at the Thomas Jefferson National Accelerator Laboratory. We also present Year II research plans using this emerging simulation capability, and discuss commercialization strategies for the vacuum electronics, plasma processing, and fusion R&D fields.

What is Integrated Multiple Effects?

- Plenty of 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
- ***multiple effects*** problems typically require coupling vers 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 (Multi-pacting - staying cryogenic)
- y modeling tools have the general solver capability needed ***ntegrate*** these. Only Tech-X's VORPAL includes particle ulation, and was already used for NP accelerator research.

VORPAL was not yet a multiple effects tool … so Goal of Project is to:

Evolve VORPAL into an Integrated Multiple Effects Tool, useful for NP accelerator modeling and design.

- Through a CRADA collaboration with researchers at the Thomas Jefferson National Accelerator Facility (JLab), provide useful and immediate application of the new capability. And V & V as well.

- Lay groundwork for the Commercial realization of integrated EM-&-Plasma-&-Thermal, which we think will be our niche for this produce. (In addition to NP accelerators, there is known interest from plasma processing and vacuum electronics industries.)

Program Status: Scheduling

- 2nd year of Phase II started Aug 13.
- 3-of-4 1st-year tasks essentially complete, with one delayed to 2nd year. One predominantly 2nd year task was started early.

	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

- Spending rate has been near optimal. (1 week late!)
- Approximately 6 personnel involved, (4 Tech-X, 2 Jlab)

Status: Two Conference Presentations

- "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).

- These presentations have jump-started our discussions with the plasma processing and vacuum electronics industry.
- At their urging, attended workshop by similar (non-plasma capable) multi-physics tools, to get ideas for user interface.

Status: We have met most Year 1 Goals

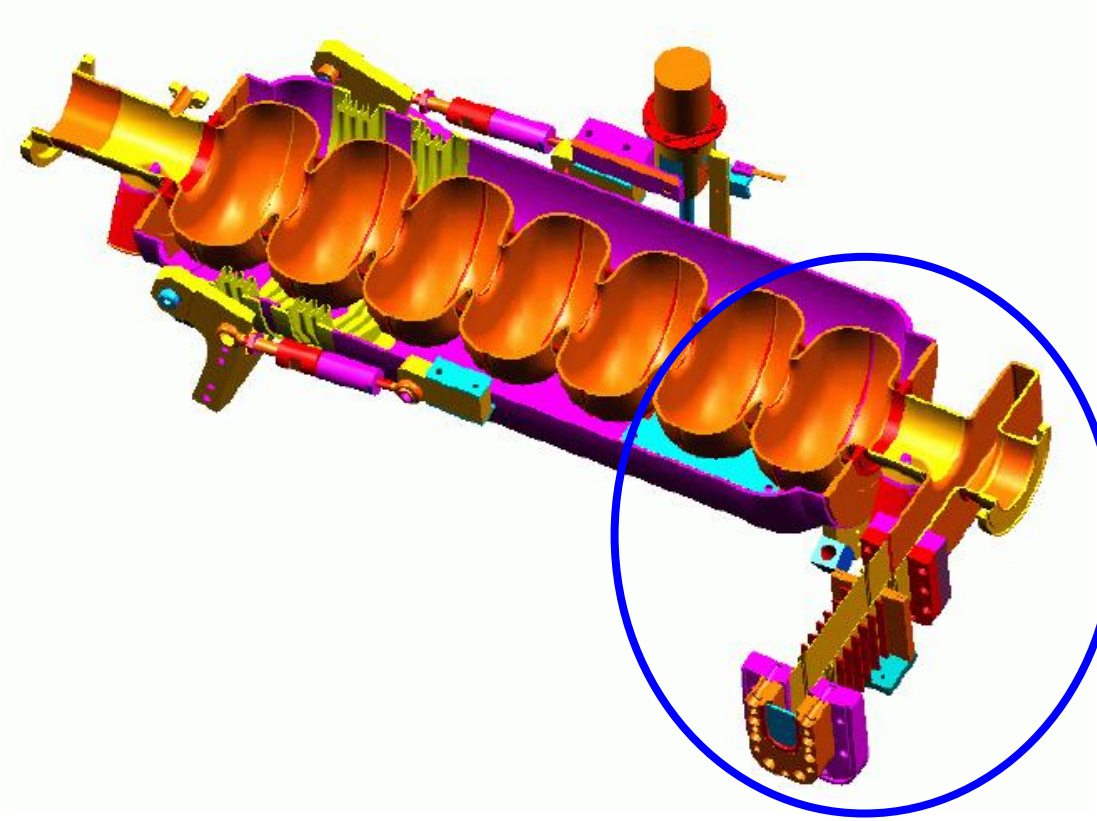
- CRADA with JLab executed, with monthly WebEx meetings.
- 3-D Cut-Cell Volume Capability added to Thermal Analysis (Task 1). √
- 3-D Cut-Cell Surface Capability is Functional, but will be optimized with more advanced algorithm in Year 2 (Task 2). √
- Thermal Benchmarking is nearly complete (Task 3).
- Geometry Primitives was started early, and is half-way complete (Task 5). √
- Advanced Materials and BC's is underway (Task 7).

(Check marks √ indicate features included in recent VORPAL 4.2 release.)

- Advanced Thermal Solver Algorithms was delayed from Year 1 to Year 2, awaiting new applied-math personnel, and will finally start around October 1 (Task 8).

A problem of interest: Superconducting RF Cavities, and HOM Couplers

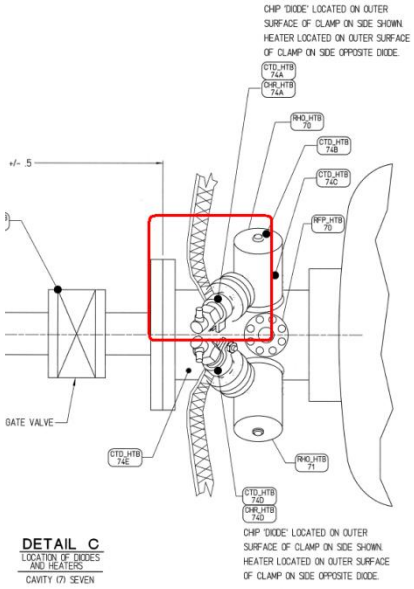
- Ohmic wall heating is a problem that combines EM and Thermal, and is the focus of most of our activity.
- High-Order-Mode couplers transition from cryogenic to normal conducting.
- Important for all cryogenic accelerators (FRIB, etc.)

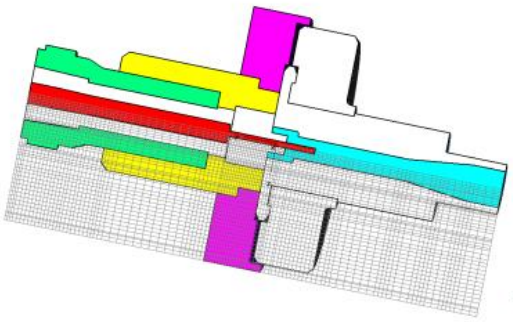


From "Design and construction of the prototype cryomodule renascence for the cebaf 12 gev upgrade," C. E. Reece, G. Ciovati, I. E. Campisi, E. F. Daly, J. Henry, W. R. Hicks, J. Hogan, P. Kneisel, D. Machie, J. Preble, T. Rothgeb, J. Sekutowicz, K. Smith, T. Whitlatch, K. M. Wilson, M. Wiseman, and G.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

Thermal Benchmarking (Task 3) is the Most Important 1st Year Task.

JLab provided a specific HOM coupler that they have measurements and previous analysis of, as well as concerns for its reliable operation.





Benchmarking has been done in 1D and 3D

- 1-D benchmarking assures proper treatment of difficult non-linear material properties. (VORPAL vs. Ansys)

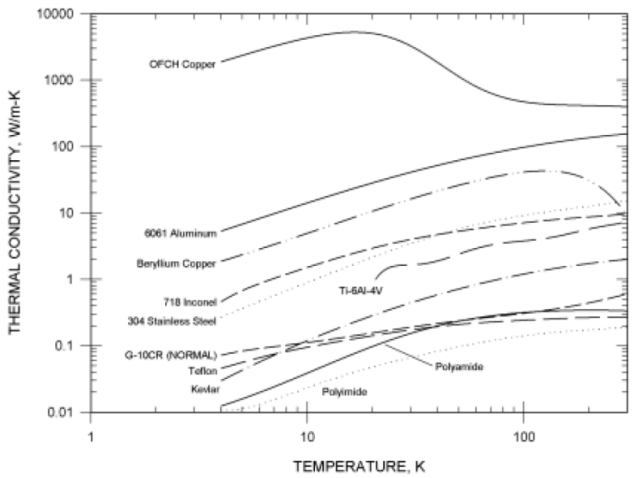
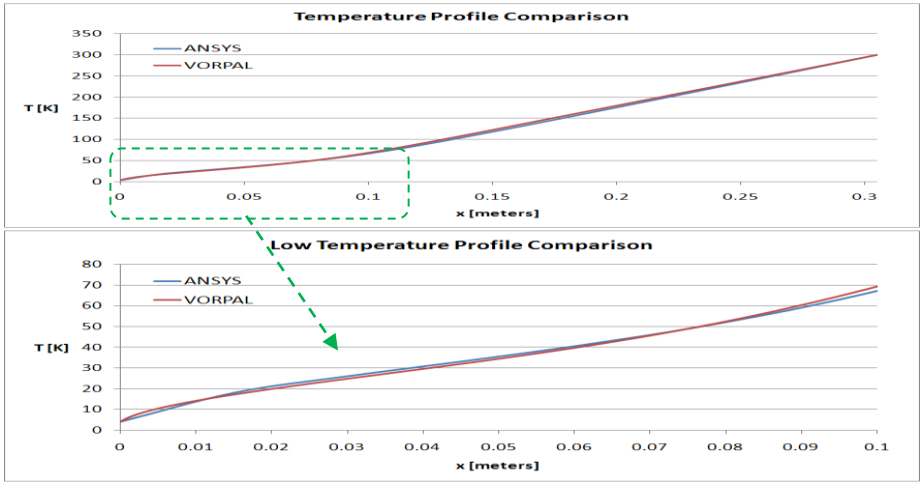
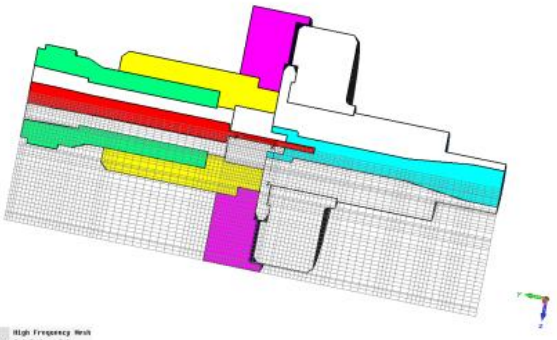
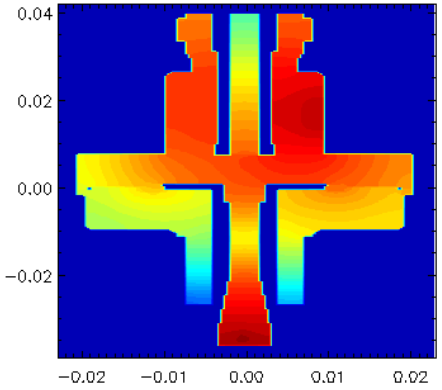


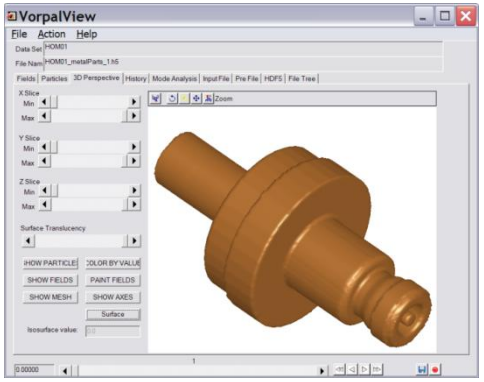
Figure 1. Thermal conductivity of various materials.



- 3-D benchmarking of various scenarios. (local heating)

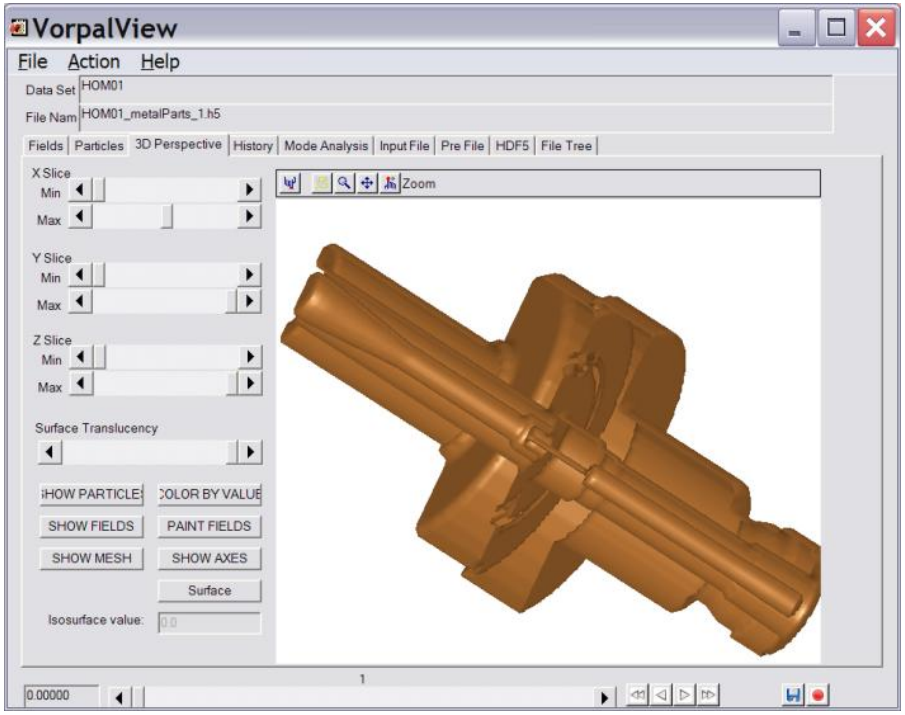


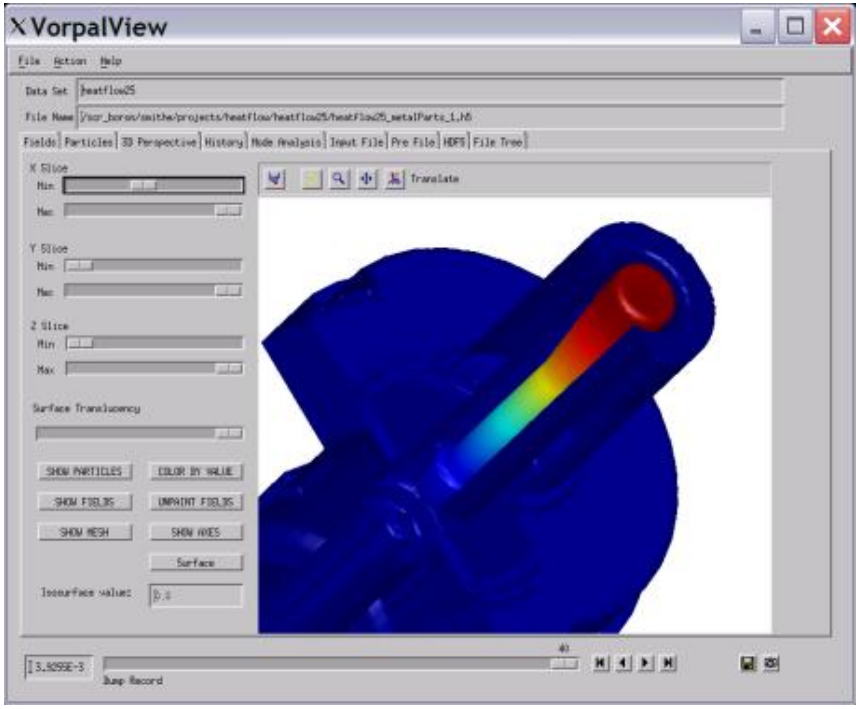




Cut-cell Thermal is new Ability (Tasks 1 & 2)

- We've done Finite Difference (FD) cut-cell EM for some time. But thermal is predominantly a Finite Element (FE) activity.
- New volume and surface element technology was added to give the ability to do true 3-D geometry thermal. Very accurate parallel resistivity. Stable to Steady-State, Dynamic in 2nd Year.





Work on Geometry Primitives (Task 5) was started early

- Primary ease-of-use task.
- Macros handle all of the (100's lines) of input file logic associated with a new part
  - Geometry description
  - Construction of thermal properties (bulk & surface)
  - Construction of EM properties (boundary conditions)
- Trying to mimic other software's (COMSOL) approaches.

```
# import CAD geometry
newCADpart(part02contact,          HOMFeedThru(02).stl, Inconel_X750)
newCADpart(part03gasket,           HOMFeedThru(03).stl, AlMg)
newCADpart(part04smallDiaSaphire,  HOMFeedThru(04).stl, Saphire)
newCADpart(part06TypeNadapter,     HOMFeedThru(06).stl, SS_304)
newCADpart(part07portTube,         HOMFeedThru(07).stl, Nb_RG)
newCADpart(part08interiorFlange,   HOMFeedThru(08).stl, Nb55Ti)
newCADpart(part09sleeve,           HOMFeedThru(09).stl, Cu_OFE)
newCADpart(part10exteriorFlange,   HOMFeedThru(10).stl, SS_316L)
newCADpart(part11bigDiaSaphire,    HOMFeedThru(11).stl, Saphire)
newCADpart(part12probeTip,         HOMFeedThru(12).stl, Nb_RRR)
```

- Year 2, connect macros to GUI (VORPAL Composer).

What's in Store for 2nd Year?

- Benchmarking ⇒ Design Modeling at JLab (Task 3).
- More materials for more problems (laminates) (Task 6).
- More boundary effects (coolant film coefficient, particle / plasma heat sources) (Task 7).
- Dynamic thermal modeling (cryogenic quench) (Task 8).
- Additional multi-physics (nonlinear magnetic material for iron shielding of earth's B-field) (Task 9).

Looking towards the Future: Lots of other potential Multi-physics Work

- Expect lots 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).

Commercialization and Use Strategy

- AES (user), Niowave (planned consult) already users in the accelerator area.
- Used in DOE Scientific Discovery (SciDAC) programs. "All DOE collaborators get to use tools for free, at the DOE computational facilites."
- VORPAL is an existing product, so there is existing marketing framework for incremental introduction of its new broadened scope to old and new customers.
- There is existing familiarity with vacuum electronics .
- Existing work with plasma processors.

Quick Summary

- Project is mostly on task, on schedule, with two tasks swapping from Year 1 to Year 2.
- JLab CRADA collaboration moving from benchmarking to design modeling in Year 2.
- Good benefit for Nuclear Physics accelerators, and good commercialization potential.