INTEGRATED EM & THERMAL SIMULATIONS WITH UPGRADED VORPAL SOFTWARE *

D. Smithe, Peter Stoltz, Dan Karipides, Tech-X Corporation, Boulder, CO 80303, U.S.A.
H. Wang, G. Cheng#, Jefferson Lab, Newport News, VA 23606, U.S.A.

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 is affected by the temperature-dependant surface resistance and in turn affects the cryogenic thermal conduction problem. Integrated EM & thermal analysis of this difficult non-linear problem is now possible with the VORPAL finite-difference time-domain simulation tool. We highlight thermal benchmarking work with a complex HOM feed-through geometry, done in collaboration with researchers at the Thomas Jefferson National Accelerator Laboratory, and discuss upcoming design studies with this emerging tool. This work is part of an effort to generalize the VORPAL framework to include generalized PDE capabilities, for wider multiphysics capabilities in the accelerator, vacuum electronics, plasma processing and fusion R&D fields, and we will also discuss user interface and algorithmic upgrades which facilitate this emerging multiphysics capability.

THERMAL UPGRADES FOR VORPAL

The Vorpal simulation software [1], widely used for electromagnetic and plasma physics modelling of nuclear and high energy accelerators, has undergone a significant upgrade over the past year, and can now perform realistic thermal modelling simulations, and can couple electromagnetic and thermal modelling in self-consistent manner. The evolution of this capability is illustrated in Figure 1, which compares the thermal modelling capability 18 months ago to present capability. Earlier thermal capability was based upon application of Vorpal's newly created generic PDE solver capability, involving gradient and divergence vector calculus operations. Such generic capability permitted only simple boundaries aligned with the computational mesh, with uniform material properties, as shown in the left panel of Figure 1.

In the past year, the general PDE capability has been integrated with more advanced non-linear material capability, and a finite-difference cut-cell thermal algorithm has been invented, following techniques previously used to create the cut-cell electromagnetic capability. Further integrations with Vorpal's CAD-based geometry engine give finally, a full-featured part-based thermal modelling capability, as illustrated in the right panel of Figure 1. Furthermore, the thermal solver retails its foundation in Vorpal's original general PDE solver capability, and so maintains its large-scale parallel computing heritage, thus being capable of very large problem size, and good parallel scaling.

The part being modelled in Figure 1 is a coaxial HOM coupler feed-through [2], under evaluation at the Jefferson Lab. This part is being studied with several electromagnetic and thermal software packages, including Vorpal, and comparison of results with other software packages, and laboratory measurement serves to benchmark the new thermal modelling capability.

HOM COUPLER BENCHMARK

A detailed description of the coaxial HOM coupler

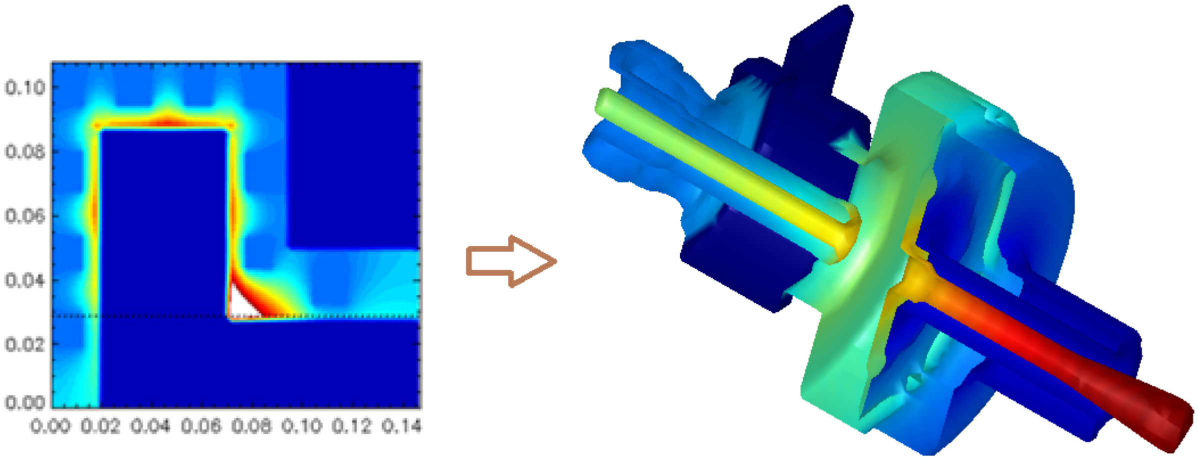


Figure 1: Illustration of the evolution of thermal modelling capability in the VORPAL software over the last 18 months, from simple hand-drawn shapes and uniform material properties, to sophisticated multi-part CAD-based geometry, with wide ranging non-linear material properties.

feed-through shown in Figure 1, and its location and function on the accelerating cavity, is provided in paper TUP107 of this conference, entitled "RF-thermal combined simulations of a HOM coaxial coupler," by G. Cheng, et. al. The axi-symmetric part of the feed-through configuration consists of 12 subparts, illustrated as the different coloured items in the cross-section Figure 2. Each of these parts is detailed in an STL-formatted CAD file, which provides geometry input. Additional items were added by hand, including a thermal clamp and strap, and coaxial extensions near the probe tip, to arrive at the 3D geometry illustrated in Figure 1.

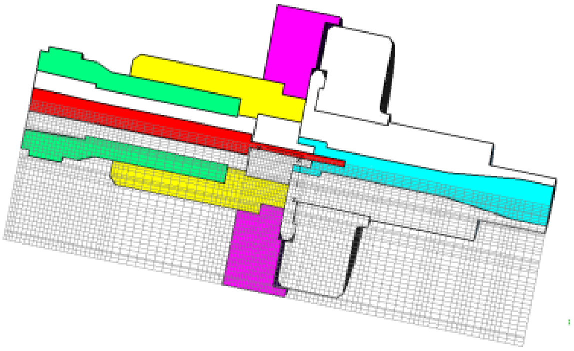


Figure 2: Cross section showing the various parts comprising the HOM coaxial feed-through.

The various parts consist of eight widely different materials: Inconel X750, AlMg, saphire, 304 stainless, niobium, niobium-alloy, and OFE copper, and each part is modelled with proper thermal conductivity, *k*. Some of these materials, copper in particular, have very non-linear behaviour in the cryogenic range, where *k*(T) varies dramatically with temperature. Different configurations of fixed-temperature and fixed heat sources are applied to the various surfaces, and a steady-state solution is achieved through forward-Euler iteration in a pseudo-time variable. Each iteration update re-evaluates the thermal conductivity, to achieve the proper non-linear *k*(T) behaviour.

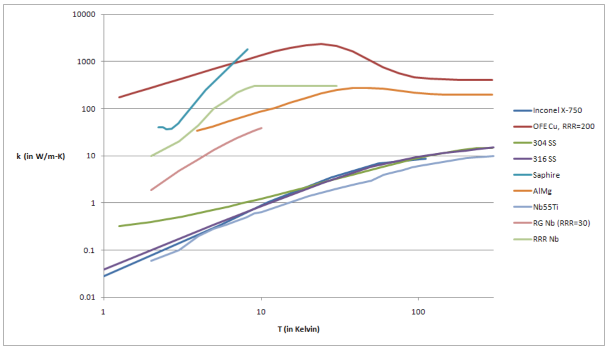


Figure 3: The challenging five-decade range of thermal conductivities for the various subpart materials in the coaxial HOM feed-through.

To date the pseudo-time iteration is optimized for fast convergence to steady-state. However work is underway to perform an implicit backward-Euler iteration, with the goal of performing actual time-dependant thermal behaviour, and in particular, a quench event. The principal computational challenge is presented by the range of thermal conductivities of the various different materials which range over nearly 5 orders of magnitude. This range of *k*(T), for temperatures between 1 and 100 K are shown in Figure 3. Solution convergence is not actually dependant on the overall range, but rather by the greatest change in *k* from one subpart to another at the part interfaces. Thus, convergence is dominated by the copper-stainless and sapphire-stainless interfaces.

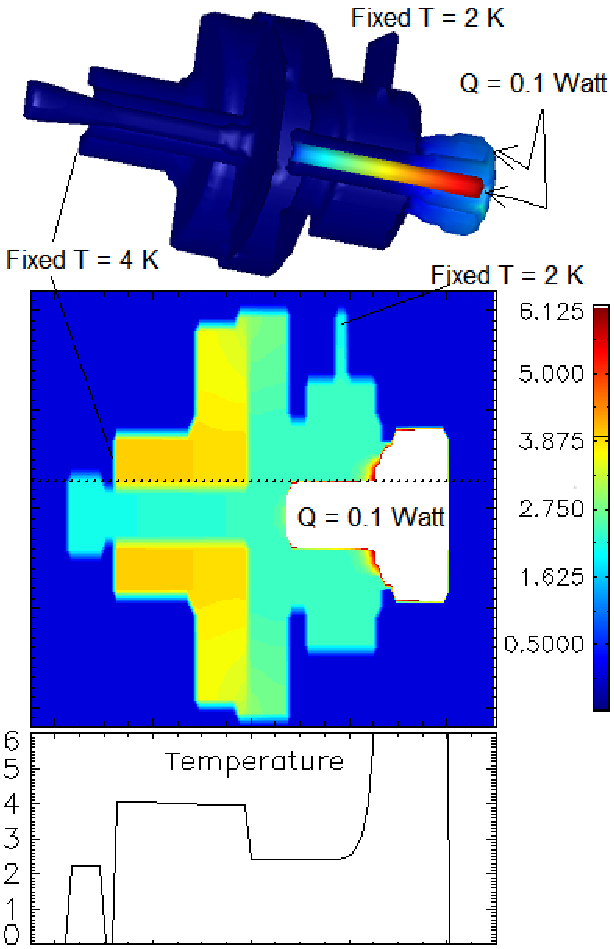


Figure 4: Thermal benchmark case based on thermal leakage back to the cryogenically cooled HOM coupler. The center coax heats to near 100 K, but the sapphire bushing and copper thermal clamp preserve the cryogenic temperatures at the probe end.

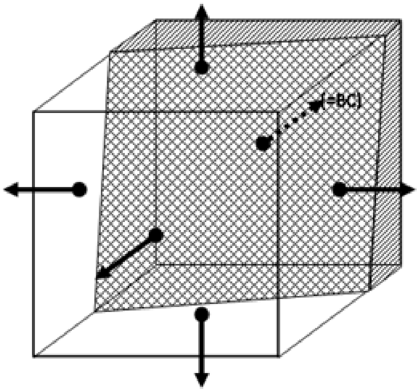
Details of the electromagnetic benchmark case are presented in paper TUP107. This same configuration is being studied as a thermal benchmark case. The principal interest is thermal leakage from the coax back to the cryogenically cooled HOM coupler. In this scenario, the end of the thermal strap is fixed at 2 K, while the probe housing is fixed at the nominal cavity temperature of 4 K. A heat source of 0.1 watts is applied to inner and outer coax of the Nadapter of the coax. The inner coax is seen to heat markedly, to 100k, however the copper thermal clamp and strap, connected to a 2K heat station, isolate the heat flow, and prevent the cryogenic material from rising above 4 K.

Additional benchmarking with this scenario is ongoing, and includes simultaneous treatment of the EM ohmic heating, as well as the static heat load from the coax line, with particular attention to scenarios and power levels that could lead to quenching of the cryogenic components.

MULTIPHYSICS ALGORITHMS

The use of finite-difference techniques, rather than finite-element, for a thermal calculation is somewhat novel, and is a direct consequence of the original finite-difference technique underlying the electromagnetic simulations. Identical meshing is used for both electromagnetic and thermal simulations, and of course, this facilitates information exchange between the two, temperature to evaluate surface resistance, and ohmic wall heating to drive the thermal evolution.

In terms of the original electromagnetic Yee-cell, we use cell-centered temperature, T, and face-centered heat flux vector, **Q**, which effectively is a conservative finite-volumes algorithm, which assures that the exact heat flux exiting a face from one cell enters that same face of the neighbour cell. Thermal conductivity is evaluated on the cell faces, hence each component of the $\mathbf{Q}=-k(T)\nabla T$ vector has its own *k*, unique to its face.



$$\partial_t \int CT \cdot d^3V = -\oint \mathbf{Q} \cdot d\mathbf{A}$$

Figure 5: Cut-cell thermal algorithm evaluates the integral of k(T) over cell surface, including cut faces composed of different material.

Furthermore, in analogy with Vorpal's Dey-Mittra cut-cell electromagnetic algorithm[3], an advanced cut-cell thermal algorithm has been developed. We are able to reuse the face-cut-area computation that is intrinsic for Dey-Mittra electromagnetics to evaluate thermal conductivity, *k*(T), on the cut-face containing a material interface. In doing so, one may choose to favour either parallel or serial heat conduction, across material interfaces. By choosing to do a proper cut-face-area evaluation of *k*(T), we are choosing to accurately portray heat conduction parallel to the interface, while allowing larger error for heat conduction across boundaries. There are two reasons for making this choice. First, for materials of vastly different conductivity, this choice is necessary to get the heat flux correct, when heat flux is predominantly in one of the two materials at the interface. Secondly, it is realized that heat conduction normal to an interface may be further impeded by contact resistance, which we may wish to address at some future time, and at that same time we could choose to implement corrections for serial heat flow.

REFERENCES

[1] C. Nieter, J. R. Cary, P. Messmer, D. Bruhwiler, D. Smithe, "Modeling of complex geometries with the plasma simuation code VORPAL," Bulletin of the American Physical Society 50, 89 (2005).

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

[3] S. Dey and R. Mittra, "A locally conformal finite-difference time-domain (FDTD) algorithm for modeling three-dimensional perfectly conducting objects," IEEE Microwave and Guided Wave Letters, Vol. 7, No. 9, pp. 273 -275, September 1997.