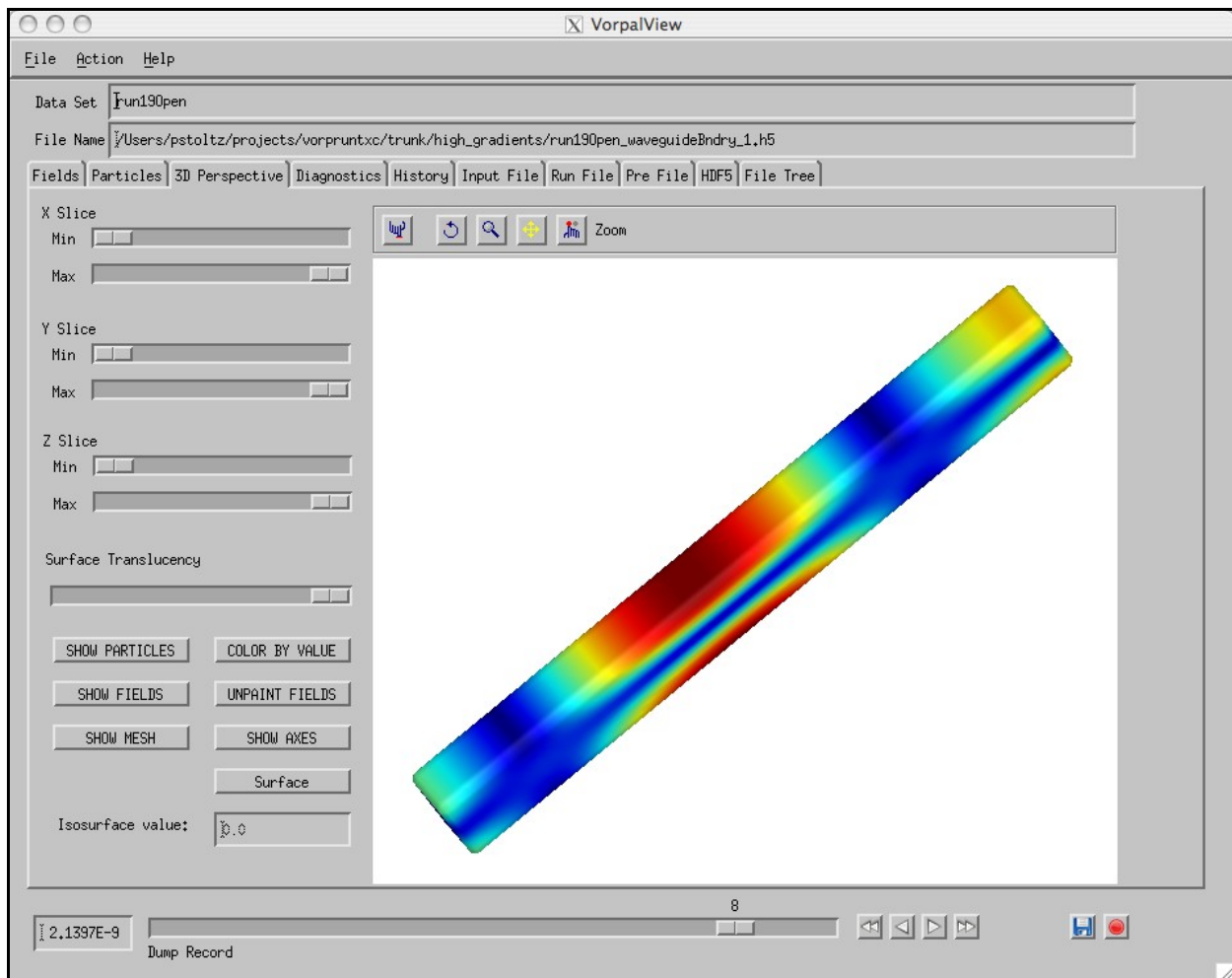


Final Report: Simulation Tools for Parallel Microwave Particle in Cell Modeling



Small Business Innovation Research Grant #: DE-FG02-03ER83841
Principal Investigator: Peter Stoltz, Tech-X Corporation
July 1, 2008



Summary

Benefit to Department of Energy:

Transport of high-power rf fields and the subsequent deposition of rf power into plasma is an important component of developing tokamak fusion energy. Two limitations on rf heating are: (i) breakdown of the metallic structures used to deliver rf power to the plasma, and (ii) a detailed understanding of how rf power couples into a plasma. Computer simulation is a main tool for helping solve both of these problems, but one of the premier tools, VORPAL, is traditionally too difficult to use for non-experts. During this Phase II project, we developed the *Vorpal/View* user interface tool. This tool allows Department of Energy researchers a fully graphical interface for analyzing VORPAL output to more easily model rf power delivery and deposition in plasmas.

Commercial Successes:

The main product of this work is the *Vorpal/View* tool for analyzing VORPAL results in a user-friendly way. This tool is used by nearly all commercial customers of VORPAL, and we believe without a user-friendly tool like *Vorpal/View*, these sales would not have been possible. Also, the physics capabilities developed under this SBIR project have led directly to increased commercial sales of the VORPAL code. Specifically, a customer in the plasma processing industry purchased a \$142,000 of commercial license and consulting for the VORPAL code based largely on the ability of the code to model deposition of rf power into a dense plasma, a feature of VORPAL vetted as part of this work.

Selected Publications and Presentation:

C. M. Roark, J. Carlsson, A. Hakim, D. P. Karipides, D. N. Smithe, P. H. Stoltz, *PIC Modeling Of Collisional Skin Depth In RF-Driven Atmospheric Pressure Plasmas*, 17th Topical Conference on Radio Frequency Power in Plasmas. AIP Conference Proceedings, Vol. 933, pp. 487-490 (2007)

P. H. Stoltz, D. N. Smithe, *Simulation of plasma effects on rf power transport in vacuum waveguides*, American Physical Society, 49th Annual Meeting of the Division of Plasma Physics, Orlando, FL, November 12-16, 2007

Selected accomplishments by task

Task 1: Improve user friendliness

The main accomplishment of this project is the *Vorpa/View* tool to allow users to examine VORPAL results with a GUI. This work was so successful that *Vorpa/View* is now the default GUI for analyzing VORPAL results and is used by nearly all VORPAL users (including almost all the VORPAL development team members). *Vorpa/View* has also made VORPAL a viable commercial product. Before this Phase II work, selling VORPAL as a commercial software tool was difficult because of the lack of a user interface. Since the completion of *Vorpa/View*, VORPAL users can easily analyze results, and this has made VORPAL easier to sell on the commercial market.

Vorpa/View is cross-platform; it runs on Windows, Mac OS X, and Linux. We accomplish this using the IDL windowing toolkit. Both *Vorpa/View* and the IDL engine that runs it are freely available. This means that collaborators do not need a VORPAL license to view VORPAL results. This is important for large collaborations, where only a few team members might have a VORPAL license, but all team members may want to view simulation results.

Figure 1 through Figure 4 show examples of the *Vorpa/View* tool. Users can examine geometries in three dimensions, and particles and fields in one, two and three dimensions. In Figure 1, we show a rectangular waveguide such as might be used in rf heating of a plasma. The color map indicates the magnetic field of a traveling wave TE₀₁ mode propagating in the waveguide. In Figure 2, we show the field viewing pane, where the user sees 1D, 2D, and 3D views of the fields. This figure shows the transverse component of electric field in the waveguide from Figure 1. The upper right pane in Figure 2 shows the 2D view, the lower right pane shows the 1D view, and the lower left pane shows the 3D view. In Figure 3, we show the time history pane. This allows users to see time histories of scalar quantities. For instance, in that figure, one sees the time history of the total number of electrons in the upper and lower windows and the time history of the total number of ions in the center window. The number of electrons is decreasing slightly, meaning electrons are being lost. The number of ions is growing, meaning ionization is taking place. Finally, Figure 4 shows how *Vorpa/View* helps users improve workflow by displaying metadata about the simulation, including the time and date the simulation was run, the version of VORPAL used, the location of the executable, and the total run time.

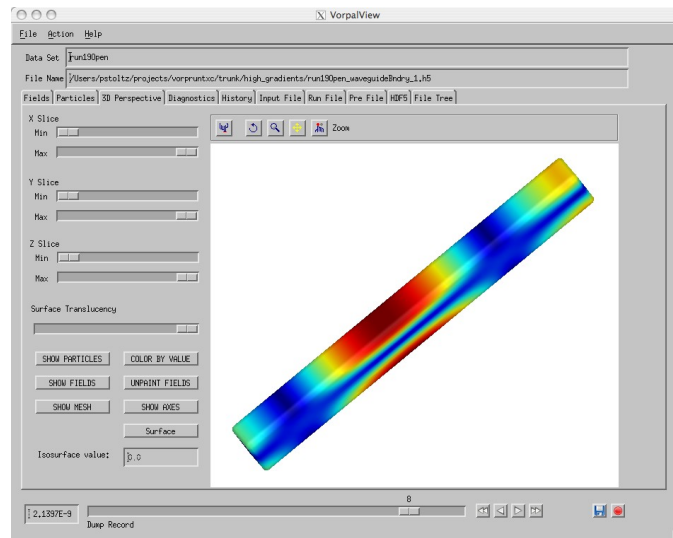


Figure 1: The VorpaiView tool is the main result of this Phase II work. VorpaiView is the standard graphical interface for examining VORPAL output, making VORPAL easier to use for researchers and more commercially viable. The color map indicates the magnetic field of a traveling wave TE01 mode propagating in the waveguide.

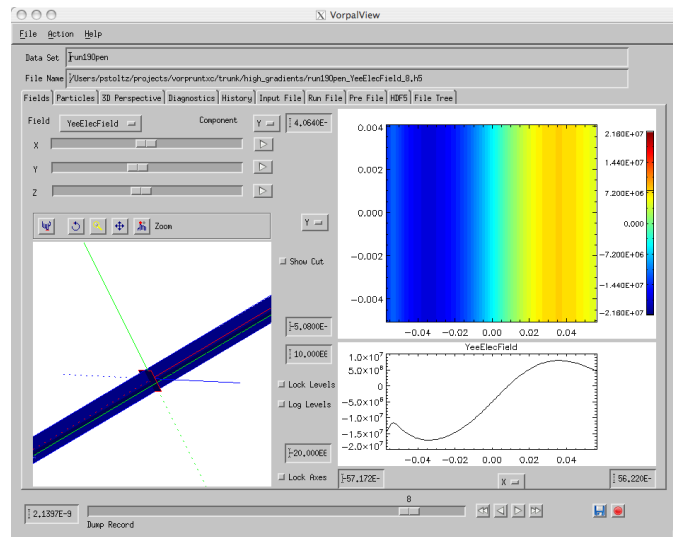


Figure 2: The VorpaiView tool allows users to inspect fields in one, two, and three dimensions.

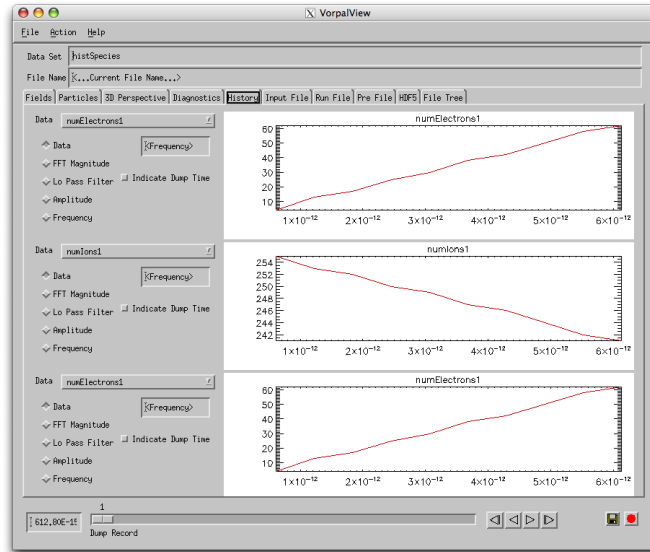


Figure 3: VorpableView allows users to examine time histories of user-selected quantities. VorpableView also gives users additional insight by providing further processing of these time histories with functions like FFT.

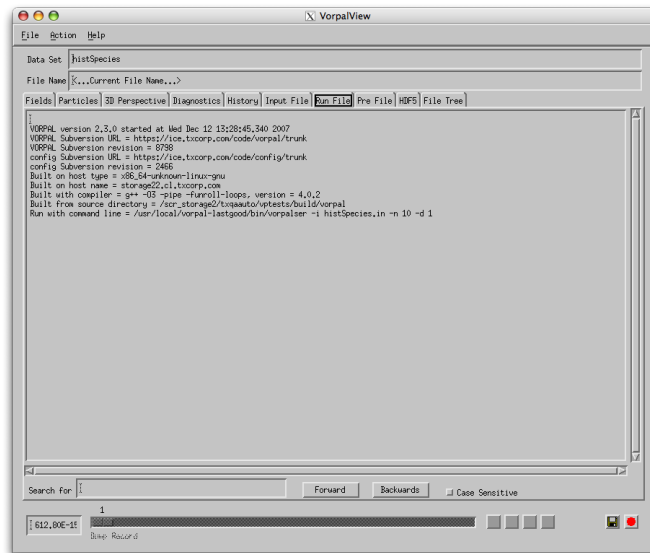


Figure 4: VorpableView improves workflow by allowing users to examine information about how VORPAL was executed.

Another part of improving the usability of VORPAL is documentation on how to use the VORPAL examples. This will make VORPAL easier to use for new users by giving detailed descriptions of how to use the VORPAL examples to model, for example, rf-plasma interaction. The documentation includes sections on what physics is modeled by each example and what VORPAL commands one needs to use those features. It also includes a Frequently Asked Questions list. Figure 5 and Figure 6 show some examples of this new documentation.

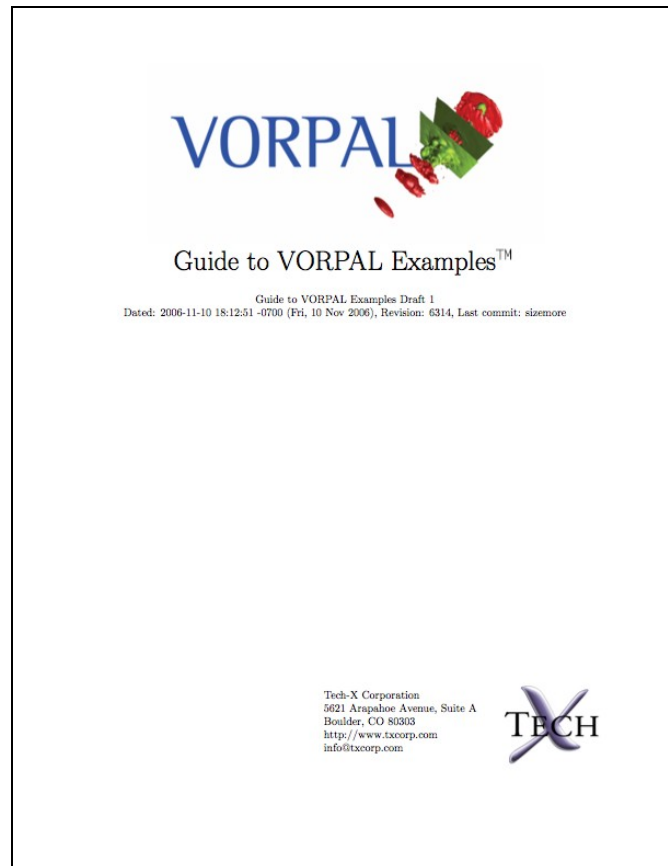


Figure 5: The new documentation we are developing. This documentation will make VORPAL easier to use for new users by giving detailed descriptions of how to use the VORPAL examples to model, for example, rf-plasma interaction.

34.4 Frequently Asked Questions

34.4.1 Are conducting boundaries required on the outside of a PML?

No. It shouldn't matter much what boundaries are put outside a PML region, but for consistency and transparency, it's better to specify the boundaries explicitly.

34.4.2 Why shouldn't I just pick a very large value for the conductivity? Won't this require fewer cells in the PML?

The PML region is perfectly matched to vacuum in the continuum limit; however, discretization spoils this match. The dispersion depends on the cell size, so even vacuum with $\Delta x = 1$ would not be perfectly matched to vacuum with $\Delta x = 2$. In practice, this means that shorter wavelengths (actually, larger wave-vector components normal to the PML interface) have greater reflection from a PML. To reduce this reflection, we gradually increase the conductivity.

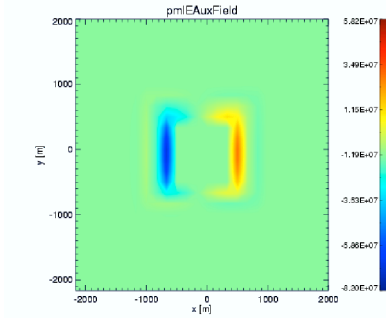


Figure 34: Sample output from eFieldBurst.

Figure 6: An example page from the new VORPAL documentation. The documentation includes sections on what physics is modeled by each example and what VORPAL commands one needs to use those features. It also includes a Frequently Asked Questions list.

Task 2: improve specification of computational grid

A main accomplishment for this task is the addition of the ability for VORPAL to import files from CAD tools. This ability allows VORPAL to work more seamlessly with experimentalists designing microwave system, as these experimentalists typically design in a CAD tool. The capability to read CAD files for geometry descriptions is also important for commercial customers.

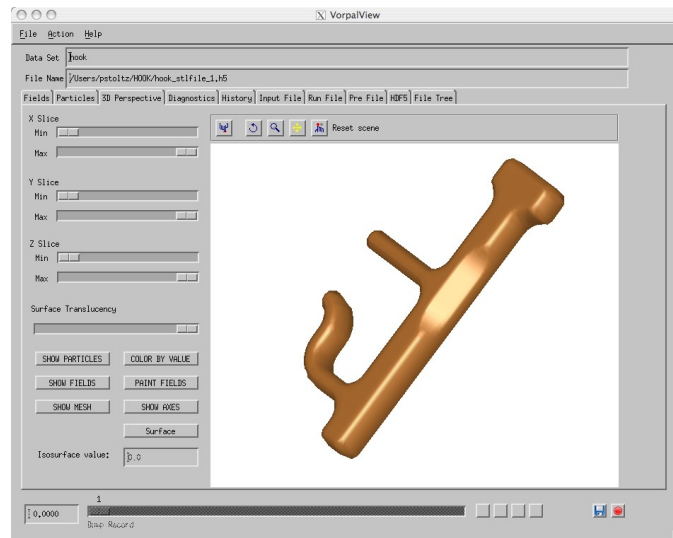


Figure 7: The ability to read CAD files as input to VORPAL is a main accomplishment of this project. This ability is important to both DoE researchers and to commercial customers.

In Figure 7 we show an example of a VORPAL simulation using geometry based on CAD. This example shows a filter for selecting certain electromagnetic modes for damping.

We show the VORPAL syntax to include a CAD file here to demonstrate how this ability makes geometry specification easier for the user. Specifying geometry based on a CAD file requires only four lines.

```
<GridBoundary stlfile>
kind = cadGridBndry
filename = hook_export.stl
</GridBoundary>
```

Presently VORPAL can include CAD files of STL format only.

Task 3: modeling microwave transmission

We completed this task successfully. A main validation effort during this project was comparison of breakdown data from Stanford Linear Accelerator Center (SLAC) for transport of high power microwaves to VORPAL simulation results. The data from SLAC is part of a collaboration including the Massachusetts Institute of Technology group of Richard Tempkin and directly relates to high power microwaves for tokamak heating. We show the setup of the data and simulations in Figure 8 and Figure 9. We show an example of the SLAC data for breakdown in Figure 10, and results of a VORPAL simulation of that

breakdown in Figure 11 and Figure 12.

Figure 11 shows VORPAL simulation results for the waveguide setup in Figure 8 with parameters based on the experiment with results shown in Figure 10. The blue line is the simulated voltage at the waveguide input (this is equivalent to the sum of black and green shown in Figure 10), and the red line is the simulated voltage at the output (equivalent to red in Figure 10). A main result is that the time to zero out the power (the red line in both Figures 10 and 11) is roughly equivalent in both simulation and experiment.

Another main result is that the spot sizes of craters required to create the neutral gas shown in Figure 12 is on the order of the craters seen in experiment, providing increased confidence in the code.

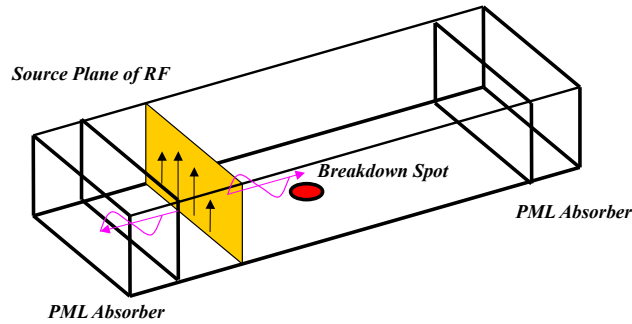


Figure 8: The setup for VORPAL simulations of waveguide breakdown.

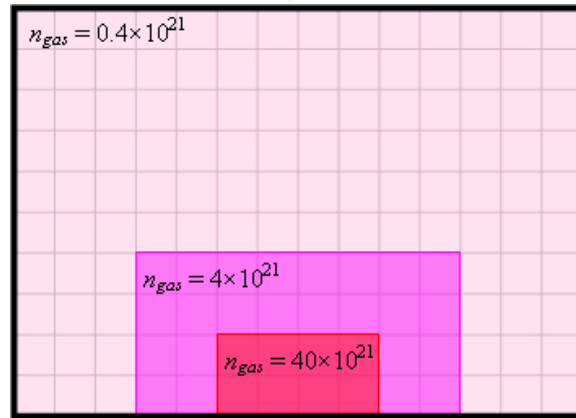


Figure 9: The assumed neutral gas density in the simulations at the plane of the hemispherical spot in the figure above. This gas density pattern mimics an expanding cloud.

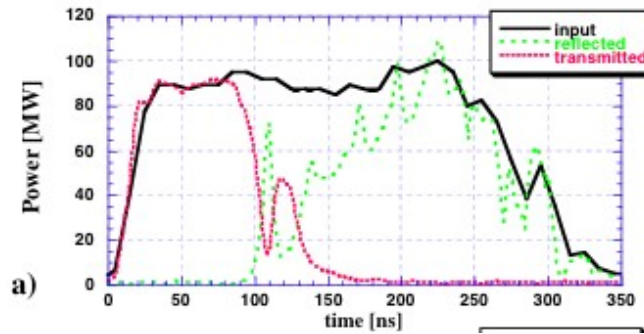


Figure 10: Measured power levels in a typical SLAC waveguide breakdown event. The black line is input power, the red line is transmitted power, and the green line is reflected power.

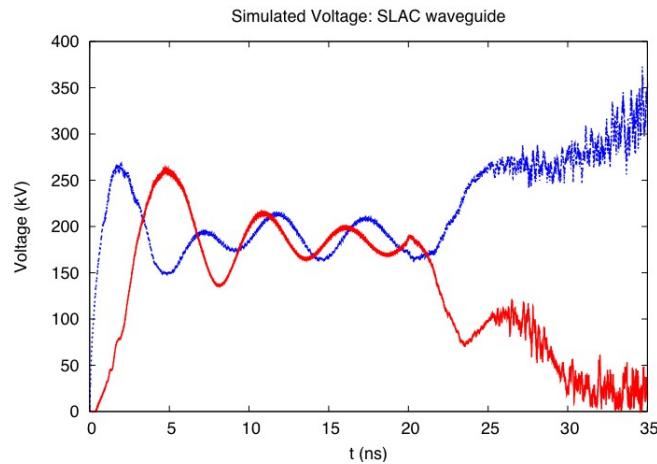


Figure 11: VORPAL simulation results for the waveguide setup shown in Figure 8 with parameters based on the experiment with results shown in Figure 10. The blue line is the simulated voltage at the waveguide input (this is equivalent to the sum of black and green shown in Figure 10), and the red line is the simulated voltage at the output (equivalent to red in Figure 10).

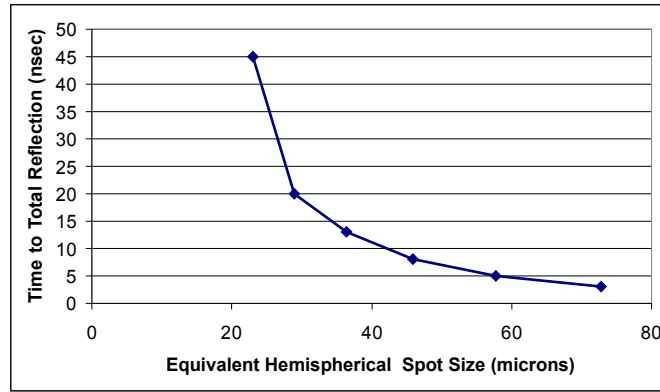


Figure 12: The simulated breakdown time as a function of assumed crater size. The SLAC experiments show roughly 100ns to total reflection. Thus, our simulations predict crater sizes less than 20 microns. This is consistent with the craters SLAC researchers see in actual waveguides.

Task 4: Improved particle emission algorithms

We completed this task successfully by adding field emission algorithms based on the Richardson-Dushman equation to VORPAL. In Figure 13, we show the current density in amps per square meter versus electric fields in the range 0-10 MV/m. These are electric field values typical of rf systems for plasma heating. This model of current emission was used in the simulations of rf breakdown in waveguides discussed above.

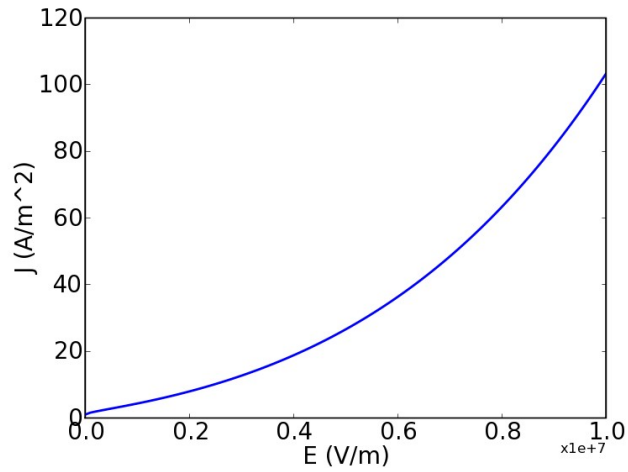


Figure 13: The emitted current density as a function of electric field strength assuming a Richardson-Dushman model of field emission. We implemented this model in VORPAL as part of this Phase II work.

An example of how to use this emitter within VORPAL is given below. The specification `emitType=2` refers to this Richardson-Dushman model.

```
<ParticleSource ParticleSourceUp0>
  kind = fieldEmitterVW
  emitType = 2
  temperature = 1000.0
  lowerBounds = [ CL_XMIN CL_YMIN CL_ZMIN]
  upperBounds = [ CL_XMAX CL_YMIN CL_ZMAX]
  direction = [0. 1. 0.]
  applyTimes = [ELECTRONTBGN 1.]
  ptclsPerStep = 100
  <NAFunc velocitySequence_0>
    kind = randGauss
    mean = 0.
    sigma = 0.
  </NAFunc>
  <NAFunc velocitySequence_1>
    kind = randGauss
    mean = VPTCLS_UP
    sigma = VPTCLS_SIG
  </NAFunc>
  <NAFunc velocitySequence_2>
```

```
    kind = randGauss
    mean = 0.
    sigma = 0.
</NAFunc>
<STFunc weightFunc>
    kind = constantFunc
    function = constantFunc
    amplitude = 1.
</STFunc>
<STFunc macroDensFunc>
    function = constantFunc
    amplitude = 1.
</STFunc>
</ParticleSource>
```