DOE Plasma Science Center

Visiting Graduate Student/Post Doctoral Researcher Fellowship Report

Title of Project:	**nonPDPSIM Training Visit**
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Host:	**Dr. Mark Kushner**
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Dates of Visit:	**Start: 6/3/13 End: 6/7/13**

I. Description and Importance of Research Issues Investigated During Visit

After several months of self-training with nonPDPSIM, there were several more complicated issues whose resolution required more in-depth instruction. As with any tool, there are non-documented techniques which will increase the productivity. Working with Natalia Babaeva and Andy Xiong allowed me to quickly learn these techniques. Previous to my visit, the settings in nonPDPSIM led to run times much greater than feasible along with non physical characteristics in the results.

Issues which were causing significant errors or problems prior to the trip included:

- Total run times longer than 6-8 weeks
- Over-predicted current (100A vs. 10A) with experimental voltage
- Boltzmann Solver output not in line with experimental results for N2
- Small numerical issue on the center line of axisymmetric cases

Without resolution of these issues, use of nonPDPSIM for the study of nanosecond pulsed discharges common in the Non-Equilibrium Thermodynamics Laboratory would be severely limited, eliminating our ability to model the plasmas in 2D in the near future.

II. Discussion of Research Outcomes and Findings Resulting from Visit

The trip led to significant progress in several issues regarding the running of nonPDPSIM.

Through building a better understanding of the plasma module ODE solver, changes in the time step settings allowed for a speed up of anywhere from 5 to 20 times. This result stemmed from depending on the iterative Jacobi solver to converge to the future time step state rather than depending on small time steps to limit the iterative solver iterations. This change increased the time step during the plasma pulse by an order of magnitude while only doubling or tripling the work done by the Jacobi solver, leading to a net overall speedup of the code.

After the pulse, the code can be sped up even more drastically using the pulsed plasma module, which turns off many of the more computationally intensive solvers, leaving only the neutral chemistry, diffusion or fluid, and energy equations. Without the Poisson solver and the plasma chemistry (such as electron impact processes) the time steps taken by the code increase in size along with the computations required per time step decreasing can decrease the run time of the code during the afterglow of the plasma by a significant factor. With these changes it is expected that the afterglow of the plasma (10ms) can be simulated in approximately the same amount of computer time as the plasma pulse (250ns).

During the visit I also received an introduction to the fluid module built into nonPDPSIM, which incorporates a compressible Navier-Stokes solver. This module provides the most accurate way to solve the energy equation, along with handle neutral species convection. Not only will this increase the accuracy of the code, but it will increase the cases for which we can use it. In many of our plasmas, some small flow is introduced to control the initial conditions of the plasmas and increase consistency of results. The fluid module will help to incorporate these effects, increasing the accuracy of the simulations.

Another result of the trip was a redesign of the circuit implemented in the circuit module. Previously the experimental voltage pulse measured across the electrodes was used, with a circuit that very nearly resembled a wire (small resistance and large capacitance). The changes included applying the non-breakdown voltage to the exterior of the simulated circuit and reproducing the pulser circuit elements within the module. While this caused larger errors in the applied gap voltage since we were no longer directly controlling it, it greatly improved the current prediction, from a steady-state value in the hundreds of amps previously down to 6-8 amps. This change brought the total coupled energy much closer to the experiment, and with tuning of other physics, that energy can be coupled at a reduced electric field comparable to what is found in the experiments.

The final result stemming from the trip was a set of changes implemented in the Boltzmann Solver by Dr. Mark Kushner shortly after the trip concluded. The changes included adding cross-sections for the electron-impact excitation of vibrational levels 9 through 17 of N2 along with a tuning of the cross-sections to better fit experimental electron swarm parameters. These changes will help the code predict both breakdown voltage and spatial reduced electric field distributions, increasing the accuracy of the relative excitation levels of different states.

III. Follow-up to Visit

After this trip, the Non-Equilibrium Thermodynamics Lab is much closer to being able to model nanosecond pulsed discharges in 2D. This ability will lead to a better understanding of vibrational excitation in N2 discharges, along with the study of plasmas such as fast-ionization waves, repeatedly pulsed plasmas, and pulsed plasmas in fuel mixtures. The progress made during this trip will allow for work such as adding the N2 master equation for V-V and V-T energy transfers to occur more quickly than it would have previously.