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Zachary D. Barker: Final DHS HS-STEM Report

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September 10, 2008

Working at Lawrence Livermore National Laboratory (LLNL) this summer has provided a very unique and special experience for me. I feel that the research opportunities given to me have allowed me to significantly benefit my research group, the laboratory, the Department of Homeland Security, and the Department of Energy. The researchers in the Single Particle Aerosol Mass Spectrometry (SPAMS) group were very welcoming and clearly wanted me to get the most out of my time in Livermore. I feel that my research partner, Veena Venkatachalam of MIT, and I have been extremely productive in meeting our research goals throughout this summer, and have learned much about working in research at a national laboratory such as Lawrence Livermore. I have learned much about the technical aspects of research while working at LLNL, however I have also gained important experience and insight into how research groups at national laboratories function. I believe that this internship has given me valuable knowledge and experience which will certainly help my transition to graduate study and a career in engineering.

My work with Veena Venkatachalam in the SPAMS group this summer has focused on two major projects. Initially, we were tasked with an analysis of data collected by the group this past spring in a large public environment. The SPAMS instrument was deployed for over two months, collecting information on many of the ambient air particles circulating through the area. Our analysis of the particle data collected during this deployment concerned several aspects, including finding groups, or clusters, of particles that seemed to appear more during certain times of day, analyzing the mass spectral data of clusters and comparing them with mass spectral data of known substances, and comparing the real-time detection capability of the SPAMS instrument with that of a commercially available biological detection instrument. This analysis was performed in support of a group report to the Department of Homeland Security on the results of the deployment.

The analysis of the deployment data revealed some interesting applications of the SPAMS instrument to homeland security situations. Using software developed in-house by SPAMS group member Dr. Paul Steele, Veena and I were able to cluster a subset of data over a certain timeframe (ranging from a single hour to an entire week). The software used makes clusters based on the mass spectral characteristics of the each particle in the data set, as well as other parameters. By looking more closely at the characteristics of individual clusters, including the mass spectra, conclusions could be made about what these particles are. This was achieved partially through examination and discussion of the mass spectral data with the members of the SPAMS group, as well as through comparison with known mass spectra collected from substances tested in the laboratory. In many cases, broad conclusions could be drawn about the identity of a cluster of particles.

Interestingly, some clusters of particles observed by the SPAMS instrument displayed periodic behavior. Preliminary conclusions could be made about the identity of particles in a given cluster, as well as the cause of the cluster's periodicity, based on a comparison of various particle data with data of known substances and contextual information about when the data was collected. For example, information about the time of day when a large influx of similar particles occurs can be used to determine whether that increase in particle count can be attributed to a certain periodic daily event. When this information is compared to information collected by the group about routine cleaning and maintenance operations, more conclusions about the identification of particle clusters can be made using this contextual information to determine if a certain particle type can be logically and reasonably linked to a certain periodic event.

Some of the analyzed particle cluster counts observed by the SPAMS instrument were also compared to information from a commercially available bio-detection instrument, deployed alongside the SPAMS instrument. Alarms from the commercially available instrument were compared to increases in particle counts of certain clusters of particles, which ultimately allowed for a more thorough analysis and identification of the types of particles that are possibly responsible for triggering alarms on the commercial instrument.

Ultimately, after analyzing the many clusters observed primarily over the first four weeks of data from the deployment, it was decided by members of the SPAMS group what information was relevant to include in the group's DHS report. Several meetings were held with the SPAMS group to evaluate the progress of the data analysis and to decide which aspects of the analysis were worth pursuing. Eventually, separate particle clusters were deemed by the group to be similar and were combined into three groups for further analysis over the first four weeks of data. The presence and periodicity of these groups over the initial four weeks of deployment were studied and presented to the SPAMS group, along with information obtained earlier in our analysis about the possible identities of particles comprising these various clusters.

Apart from the analysis of data collected earlier in the year by the SPAMS group, Veena and I were also given the opportunity to use the SPAMS instrument for a separate research project involving pesticide detection. The SPAMS instrument has previously been used in research by SPAMS group member Audrey N. Martin, a Ph.D. candidate at Michigan State University, with whom Veena and I worked closely during our internship. Audrey has shown previously that the SPAMS instrument is capable of detecting single particles of high explosives, chemical weapons simulants, and pharmaceuticals in real time. Our research this summer has demonstrated that the abilities of the SPAMS instrument can be extended to pesticide detection in a variety of situations.

The initial phase of pesticide research involved selecting a number of pesticides on which to focus our research. After analyzing several options, a set of five different pesticide compounds, representing four different chemical classes, was selected for research using SPAMS. These pesticides are varied in chemical and physical properties, as well as their uses in the home and in agriculture. The list of pesticides includes permethrin (pyrethroid class), dichlorvos and malathion (organophosphate class), imidacloprid (chloronicotinyl class), and carbaryl (carbamate class). Each pesticide was tested using the SPAMS instrument, producing mass spectral data to analyze.

The analysis of each pesticide compound provided an extremely valuable opportunity to learn about the SPAMS instrument and how to use it to successfully and efficiently conduct our research. Veena and I learned much about the technical aspects of working with research equipment simply by using it in our day-to-day work. Our mentors, Dr. George Farquar and Audrey Martin, were very accommodating and helpful in teaching us what we needed to know in order to successfully use the equipment to achieve our research goals. Although sample preparation was relatively simple (this is one of the main advantages to research with the SPAMS instrument), Veena and I were still able to apply our previously attained laboratory skills while handling and preparing our pesticide samples for analysis.

After collecting data on our pesticide samples, analysis of the data became the main priority of the research project. In most cases, thousands of mass spectra were collected from each pesticide sample. Analysis of data sets on this scale was only possible with the aid of software developed by Dr. Paul Steele of LLNL. Using this software, it was possible to view single particle spectra, averages of all spectra, and other supplemental information collected by the SPAMS instrument, such as aerodynamic sizing information and rate of spectrum collection. The analysis tools available proved to be essential in analyzing and presenting the data in a formal and consistent manner.

Our pesticide research using SPAMS also looked into the practical pesticide detection potential of the instrument. Two household items containing active pesticide ingredients, Raid™ Ant Killer 16 (containing permethrin) and a canine flea collar (containing carbaryl), were also studied using the instrument. The SPAMS instrument was demonstrated to detect the active ingredients in these items, and this was confirmed by analyzing the spectra obtained here with those of the pesticide standards. The fact that these samples were successfully analyzed with no preparation or pre-concentration of the active ingredient demonstrates the usefulness of the SPAMS instrument to many pesticide detection applications.

The pesticide research conducted this summer was the subject of a poster displayed at the laboratory's summer research symposium, and is also the subject of a scientific paper currently in progress. The paper will eventually be submitted to the journal Environmental Science and Technology for publishing.

Additionally, working at Lawrence Livermore has given me the chance to learn from many preeminent researchers outside of my research group, and has allowed me to visit some of the premier research facilities located within LLNL. The DHS lecture series was an extremely interesting opportunity for me to learn about the various research projects being conducted at the laboratory. The projects showcased in this lecture series gave the students an extremely broad look at the work being done at LLNL. Students were introduced to projects from such diverse subjects as national/global security and intelligence, radiation detection, climatology and weather forecasting, computation, network assessment, and biological preparedness/security. I feel that these lectures were very successful showing the many different ways that one can contribute to the safety and security of the United States. The efforts that are underway at LLNL, as well as at the other national laboratories, are vital to the new challenges that we face in coming years, and I believe that these lectures put the solutions to these challenges into context, and will motivate many students to put forth their own contributions in the future. Personally, I felt extremely motivated by many of the projects being described at these lectures. In particular, the projects concerning some new nuclear physics projects and current computation efforts at LLNL were especially interesting and inspiring to me and have given me a starting point for my decisions concerning graduate study and future career options.

In addition, there were opportunities for tours of the many highly specialized, world class facilities located at LLNL. I was able to attend tours of the National Ignition Facility (NIF), the Center for Accelerator Mass Spectrometry (CAMS), the Terascale Simulation Facility (TSF), and the High Explosives Applications Facility (HEAF). These buildings all house very important, large scale research efforts, and it was a tremendous advantage for the interns to get an idea of how research is conducted in these laboratory facilities.

While the National Ignition Facility is perhaps one of the most widely publicized research endeavors being conducted at LLNL, the other facilities offered some interesting insights into the other research areas that the laboratory is responsible for. In particular, the HEAF facility and the Terascale Simulation Facility appealed to my physics, engineering, and computer science interests.

The HEAF facility demonstrated current efforts in explosives design for military and industrial applications. Students were shown some of the “gun tanks” where on-site explosives testing is conducted, as well as posters highlighting some of the recent research completed by the facility’s staff. The tour also presented opportunities to ask some of the scientific staff at HEAF about their respective fields and their experiences working at the laboratory.

The Terascale Simulation Facility tour was also an interesting experience for many students, including myself. In this tour, we were shown the main computer floor, where two of the fastest supercomputers in the world, Blue Gene/L and ASC Purple, are currently housed. Contextual information about the computers located within the TSF was provided, demonstrating the importance of large-scale computing to LLNL’s mission of stockpile stewardship. Other visualizations of work done at TSF, ranging from seismic modeling to weather forecasting, were presented and explained to students.

I was also fortunate enough to be given the opportunity to attend a graduate school seminar at Sandia National Laboratory (Livermore, CA). Many of the interns at Sandia were in attendance, as well as some of my fellow interns from LLNL. Dr. Colette E. Patt from the University of California, Berkeley, presented a lecture on what graduate schools look for in applicants, and how potential graduate students can enhance their chances of graduate school admission and success. I found this seminar to be particularly useful, not necessarily for my responsibilities at LLNL, but rather in helping me plan out the next phase of my educational career and beyond.

There are numerous areas of research that could be of interest to the Department of Homeland Security. From my time at the laboratory, I saw many efforts focused on areas ranging from biological security to sustainable energy. To me, the term “homeland security” is all-encompassing. This means that in order for the United States to be considered secure, protection from physical threats should be in place, but independence and self-reliance should be strongly emphasized in order to minimize the opportunities for threats to bring harm to the nation. This especially includes areas of research such as reliable, sustainable, domestic energy platforms, such as those currently being researched at Lawrence Livermore and other Department of Energy facilities.

Additionally, areas of biological research seem to be emerging as an important area of homeland security research. Biology and genome research has fantastic potential to make significant advances in medicine, but also has important applications to the protection of public health, particularly from wide-spread biological threats. Much of the biological research being conducted at LLNL deals with homeland security issues and issues of the protection of public health, and I feel that there is tremendous potential for even more work to be done throughout the national laboratory system and at research universities.

From the start of the internship experience, it was obvious to me that the research being conducted, not just within my research group, but in the laboratory as a whole, was of immense national importance. As I wrap up my summer research experience at Lawrence Livermore National Laboratory, I feel that I have gained a new understanding of the scientific challenges that will confront the United States in the near future. After having been fortunate enough to meet and work with the many talented individuals working at LLNL, I feel confident that the United States will remain at the forefront of scientific research, and will be able to meet the scientific challenges of the present and future.