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# DHS Research Experience Summary

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November 14, 2008

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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August 2008  
DHS Research Experience Summary:  
Summer 2008, at Lawrence Livermore National Laboratory

I learned a great deal during my summer internship at Lawrence Livermore National Laboratory (LLNL). I plan to continue a career in research, and I feel that my experience at LLNL has been formative. I was exposed to a new area of research, as part of the Single Particle Aerosol Mass Spectrometry (SPAMS) group, and I had the opportunity to work on projects that I would not have been able to work on anywhere else. The projects both involved the use of a novel mass spectrometer that was developed at LLNL, so I would not have been able to do this research at any other facility.

My research advisors were George Farquar, Audrey Martin, and Matthias Frank. I had a chance to work on two projects, together with Zachary Barker, a fellow DHS intern. One project, on pesticide detection, was self-contained and fairly straightforward. The other was part of a larger analysis involving finding common compounds that could be detected in the ambient air. The technical details of these projects are summarized in more detail below.

### **Pesticide Detection Using Single Particle Aerosol Mass Spectroscopy**

The first project that Zachary and I worked on involved using SPAMS to detect pesticides. The ability to rapidly detect pesticides in a variety of matrices is applicable to many fields including public health, homeland security, and environmental protection. Real-time, or near real-time, detection of potentially harmful or toxic chemical agents

can offer significant advantages in the protection of public health from accidental or intentional releases of harmful pesticides, and can help to monitor the environmental effects of controlled releases of pesticides for pest control purposes. The use of organophosphate neurotoxins by terrorists is a possibility that has been described; this is a legitimate threat, considering the ease of access, toxicity, and relatively low cost of these substances.

Single Particle Aerosol Mass Spectrometry (SPAMS) has successfully been used to identify a wide array of chemical compounds, including drugs, high explosives, biological materials, and chemical warfare agent simulants. Much of this groundbreaking work was carried out by our group at LLNL. In our work, we had the chance to show that SPAMS fulfills a demonstrated need for a method of carrying out real-time pesticide detection with minimal sample preparation. We did this by using a single particle aerosol mass spectrometer to obtain spectra of five different pesticides.

Pesticide samples were chosen to represent four common classes of pesticides that are currently used in the US. Permethrin (a pyrethrin insecticide), dichlorvos and malathion (organophosphates), imidacloprid (a chloronicotinyl pesticide), and carbaryl (a carbamate) were selected for analysis. Samples were aerosolized either in water (using a plastic nebulizer) or in ethanol (using a glass nebulizer), and the particles entered the SPAMS instrument through a focusing lens stack. The particles then passed through a stage with three tracking lasers that were used to determine each particle's velocity. This velocity was used to calculate when to fire a desorption/ionization (D/I) laser in order to fragment the particle for analysis in a dual

polarity time of flight mass spectrometer. Signals were digitized, and then analyzed using LLNL-developed software.

We obtained chemical mass spectral signatures for each pesticide, and assigned peaks to the mass spectra based on our knowledge of the pesticides' chemical structures. We then proved the robustness of our detection method by identifying the presence of pesticides in two real-world matrices: Raid™ Ant Spray and a flea collar. To sample these, we simply needed to direct aerosolized particles into the SPAMS instrument. The minimal sample preparation required makes SPAMS very attractive as a detector.

Essentially, we were able to show that SPAMS is a reliable and effective method for detecting pesticides at extremely low concentrations in a variety of matrices and physical states.

### **Detecting Unknown Agents Using Single Particle Aerosol Mass Spectroscopy**

The other project that I had the opportunity to be a part of did not involve data collection in the lab; it consisted of analyzing a large amount of data that had already been collected. We got to look at data collected over the course of about two months, when the SPAMS instrument was deployed to a public place. The machine sampled the air and collected spectra for over two months, storing all the spectra and associated data; we then looked at an approximately two-month subset of this data to search for patterns in the types of particles being detected.

Essentially, we were able to identify particle types among all the spectra collected by clustering the spectra into groups of similar spectra. This was done using

software that had been previously developed by our group (Dr. Paul Steele, a former group member, was instrumental in helping us learn how to use the software). Once we had found particles that seemed to recur, we faced the task of trying to figure out what these particles were. To do this, we compared the average spectra for each major cluster to those of several common compounds. We were able to tentatively identify at least one compound this way.

We also looked at patterns in the appearance of different compounds. For instance, there were some compounds that only appeared at certain times of the day. Such details were interesting to note; they certainly provide the motivation for further study! In general, it was exciting to look at and think about such a large dataset...there were many different approaches to take, and coming up with the best way to interpret the data was a thought-provoking challenge. The skills I learned while analyzing this data will certainly help me in the future.

### **My Achievements at LLNL**

I think that I accomplished a lot this summer. At the end of the summer, Zachary Barker and I prepared and presented a poster on our pesticide detection work at LLNL's student poster symposium. It was an excellent venue to both meet eminent research scientists and to talk about our research with them. (The symposium also served as a way for us to familiarize ourselves with the work that the other summer interns had done, which I appreciated.) In addition to this, we drafted our pesticide work as a paper for submission to a professional journal, and will be submitting it shortly. The analysis

that we did for the project involving the detection of unknown compounds in the ambient air was contributed to the group for use in future presentations.

Overall, I think that I did much more than I could have anticipated this summer. One contributing factor to this was the overwhelming support of Audrey Martin and George Farquar in the lab. They spent a great deal of their time with Zachary and me to get us oriented, and to show us how to use the tools we needed to undertake our projects. Also, we were able to begin working almost immediately after our arrival at the lab, which was very nice; our group had several projects lined up for us, so we were never bored. Lastly, I valued the chance that I had to work on a variety of topics; I picked up skills that will inevitably be useful in the future, including learning how to analyze large data sets, and how to fix instrumentation in the lab.

### **Other Activities at LLNL**

Some of my most memorable experiences at LLNL involved going to seminars and attending tours of various Lab facilities.

One facility that I was lucky enough to visit was NIF, the nuclear ignition facility. Built with the goal of achieving fusion by focusing an unprecedented number of high-power lasers on a tiny tritium atom, the building that houses the lasers is enormous. It is built on a scale that you can only find at huge, government-funded facilities. Having a chance to see such “big science” up close was definitely not an experience that I will forget. Seeing NIF really made me aware of the crucial role that the government plays in catalyzing scientific research, and I realized how important it is for the government to continue to support such research efforts.

I also was able to visit HEAF, the high explosives research facility. As a chemist, I was particularly interested to learn about how they were developing new high-nitrogen compounds that could serve as safer explosives. These would be stable enough to not detonate by accident. Often, when we think of research on explosives as being destructive, but it is very important. Safe explosives are necessary, for example, in construction. On the tour, I learned a lot about how explosives are used, and why it is important to research them.

Another memorable facility tour was that of the Center for Accelerator Mass Spectrometry (CAMS). Here, we got to see how the concentration of trace radioactive elements in samples could be determined (among other things). This capability is very useful in radioactive dating to determine the age of various biological organisms. It can also be used in medicine, to measure when certain tissues were made, thereby giving us a sense of how the human body develops. The possible medicinal applications of accelerator mass spectrometry caught my attention; I hope to enter an MD/PhD program in the fall, and seeing that the Lab was doing research that was so connected to medicine was exciting. I could see myself doing medical work with DHS at some point in the future.

Tours were not the only way for us to get a feel for the kind of cutting edge science that is being done at the lab. We also had weekly seminars with prominent researchers at LLNL, about various topics related to homeland security. These were particularly interesting because they addressed topics that we, as Department of Homeland Security interns, were already interested in. For example, Dr. Tom Slezak discussed the viral detection platform, which shows promise as a tool that can be used



to rapidly identify biological threats. It functions by taking a sample of biological fluid from a patient, and then putting this through a series of steps that allow, ultimately, for viral DNA in the sample to be sequenced and identified.

Another speaker discussed neutrino detectors, and how the lab is working to develop better detectors. Someday, this research might be used to determine when other countries have nuclear capabilities that those countries claim not to have. There were many other interesting talks, on topics including computation (LLNL is home to the world's second fastest supercomputer), weather forecasting, and national intelligence. The seminars that we attended provided a wonderful overview of some of the really interesting work that is being done at LLNL, and I'm glad that I was exposed to so many different areas of research. I got the sense that LLNL is a very scientifically diverse place to be, and if I get to work there again, I know that there will be no shortage of interesting projects to work on.

Finally, I wanted to comment on one particular seminar that stood out for me. Dr. Farquar took Zachary and me to a talk on microcantilevers, and how they can be used as gas sensors. I am not an engineer, but listening to the talk, I began thinking about how we might use the same basic microcantilever technology in pathogen detection. The experience made me realize how the diversity of work being done at LLNL, and the closeness of the different groups, makes it very easy to draw connections across fields. LLNL encourages interdisciplinary work, which appeals to me. Noteworthy ideas are often conceived at the interface between different fields, or when someone thinks about an old problem in a new way; and from what I've seen, LLNL seems like the kind of place that fosters such innovation

Overall, my internship played a key role in my career planning. To begin with, I realized that I definitely want to do research. I also realized that I want to integrate the protection of our national interests into that research, somehow. As a DHS scholar, I feel that I am in a unique position to impact the way in which we approach the security of our nation, and at LLNL, I learned that there are a lot of different ways in which I can make an impact. I was surprised and impressed by the amount of biology being done at LLNL; I hope that, once I get my MD/PhD, I can contribute to our national biosecurity. I want to develop ways to rapidly counter the effects of a bioterrorist attack, and I think that I will be prepared to tackle this task at some point down the road, once I attend medical school.

### **Areas of research that could help DHS achieve its goals**

I gained a lot of insight into what it takes to protect a country this summer, and one belief that my experiences reinforced is that we need to continue to focus on science and technology if we want to keep our nation secure.

To be honest, I think that DHS is doing a great job of promoting research. However, the area of research that I think is most important is research on threat detection. Since the materials necessary for terrorists to cause serious damage are not as difficult to get as they once were; for example, there are molecular biology kits that will allow anyone who can pay to recombine genes in novel, potentially harmful ways. So, identifying such threats quickly will allow us to respond more effectively.

Overall, my summer at LLNL was wonderful. I met many people with whom I will certainly keep in touch, and my experience gave me a lot to think about as I move on to pursue further studies, and my career.