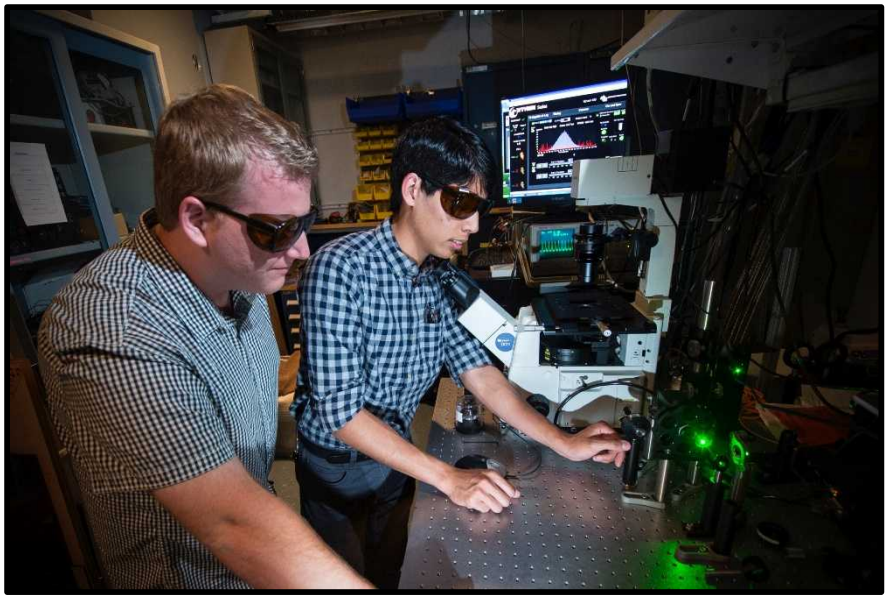
Highlights of the 2016 Summer Laboratory Student Intern Program at Sandia National Labs

Optimized Bandwidth-Compression of Ultrafast Laser Pulses

SULI participant from Sandia National Laboratories (SNL)



Mr. Emmanuel Valenton (right), a senior from the University of California, Berkeley, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"I enjoyed learning how to control laser pulses and was thrilled that I could combine that knowledge with my previous understanding of how to design data acquisition and control systems."

- Combined picosecond (10^{-12} s) and femtosecond (10^{-15} s) laser pulses can give sensitive, low-noise measurements of important quantities in reacting flows, such as species concentrations and temperature.
- Emmanuel's work focused on the development of an instrument for tailoring the time profile of picosecond laser pulses for use in nonlinear optical spectroscopic methods created from broad bandwidth femtosecond pulses. In addition to constructing the device, Emmanuel produced a LabView-based automation code, building off skills he developed in a previous CCI internship at Sandia.
- Emmanuel is now attending the doctoral program in chemistry at the University of Chicago.

Heat Transfer through Dual-Paned Windows – A Model Problem

CCI participant from Sandia National Laboratories (SNL)

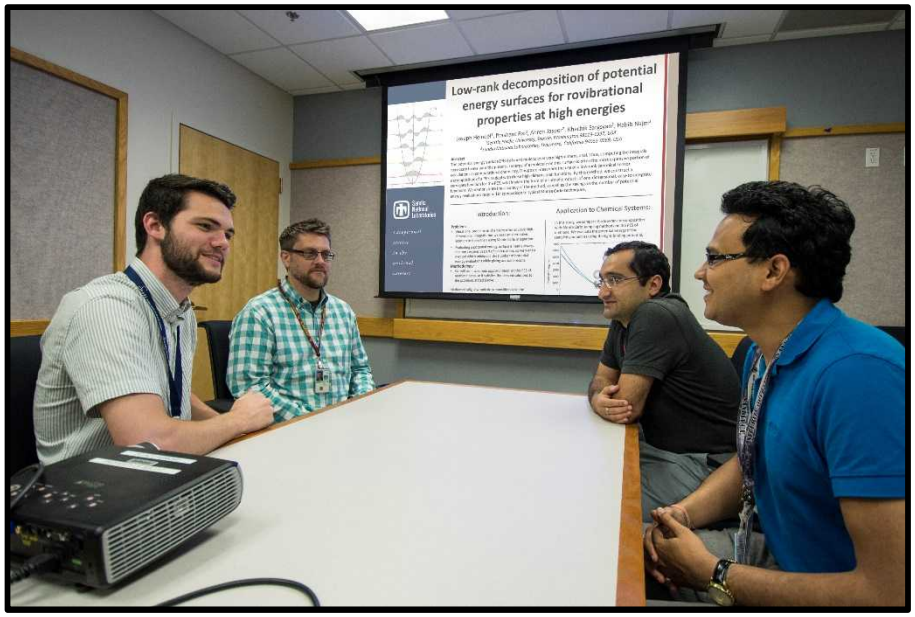
Ms. Sarah Castorena (left), a second year student from Napa Valley College, participated in the CCI 2016 Summer Term at Sandia National Laboratories.

"I found it inspiring to work around so many smart people. I also appreciated the support and advice from other interns."

- As a demonstration problem that will be included in the UQ Toolkit, a publically available set of computer algorithms and tools for performing uncertainty quantification, Sarah developed the solution for the steady-state heat flux through a dual-paned window, when allowing for uncertainties in the knowledge of the bounding temperatures and the heat transfer properties.
- To perform forward uncertainty propagation, polynomial chaos expansion with full quadrature numerical integration was performed, using Python.
- Sarah's results demonstrate the strong reduction in energy loss through dual-paned windows, the heat transfer mechanisms that most strongly influence energy loss for single-pane and dual-paned windows, and the effects of parameter uncertainty on the calculated energy loss.

Molecular Potential Energy Surfaces in Computational Chemistry

SULI participant from Sandia National Laboratories (SNL)



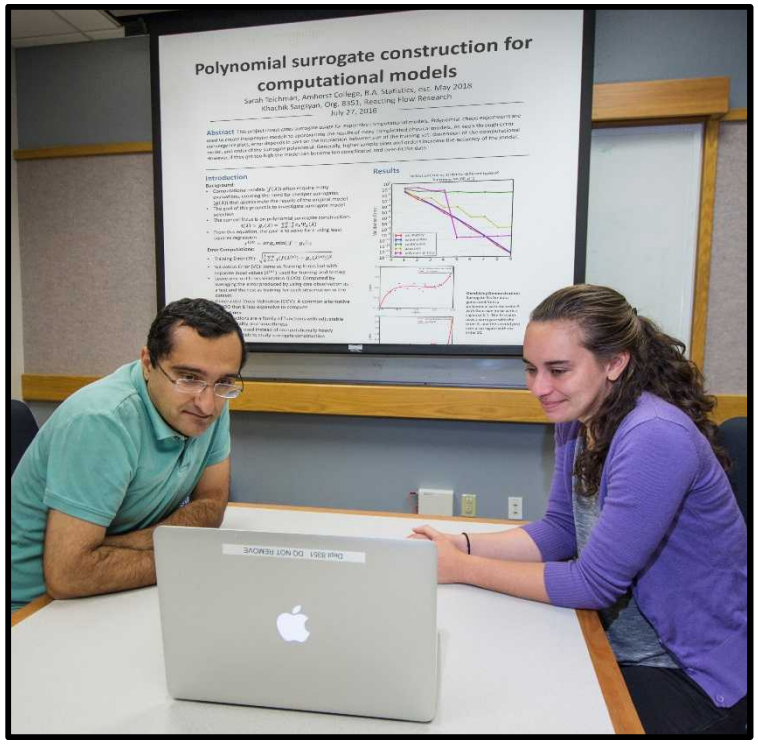
Mr. Joseph Heindel (left), a junior from Seattle Pacific University, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"With the two co-mentors that I worked with, I was able to explore the intersection of chemistry and advanced mathematical analysis."

- A common challenging issue in computational chemistry is solving high-dimensional integrals used to compute the potential energy surface of molecular systems, which in turn dictates the behavior of the molecules and how they react.
- The problem is that these integrals are very high-dimensional—meaning they depend on many different variables. To overcome this, Joseph used what is called a low-rank decomposition, which essentially takes the single high-dimensional integral one starts with and breaks it into many one-dimensional integrals which are much more tractable.
- Joseph's work demonstrated that a low-rank decomposition greatly increases the efficiency of the required calculations, which allows the computation of the potential energy surfaces for much larger systems that are important to both environmental and combustion chemistry.

Constructing Surrogate Models for Physical Systems

SULI participant from Sandia National Laboratories (SNL)



Ms. Sarah Teichman (right), a sophomore from Amherst College, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"I found working as part of a team on uncertainty quantification techniques to be very challenging and fulfilling. Now I am seriously considering going to graduate school."

- Uncertainty quantification focuses on errors in physical models: how input value noise, incorrect models, and other errors affect the variance of outputs. Certain models, including many of the complex chemical systems involved in combustion, have a high number of input parameters and are therefore computationally expensive to work with. Surrogates are simple and inexpensive models that can approximate the results of complicated physical models and thereby allow detailed evaluation of model sensitivities.
- Sarah studied surrogates constructed with a technique called polynomial chaos expansion. She investigated how certain attributes of the surrogate models affect the error between the physical model and associated surrogate.
- Sarah's work demonstrated how surrogate accuracy generally suffers as the dimension of the problem grows, but only dimensions with highly nonlinear behavior impact the convergence.

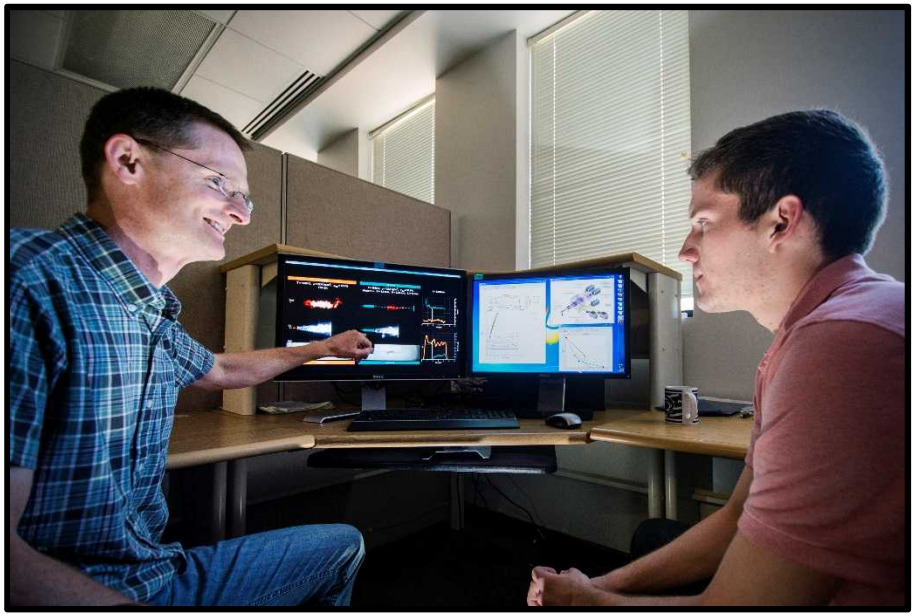
Hydrogen Production via Solar Water Splitting
SULI participant from Sandia National Laboratories (SNL)

Mr. Akash Biswas (left), a sophomore from UCLA, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"It was exciting to work on a project that could help combat global warming in a very tangible way."

- Hydrogen produced from renewable energy sources is an effective energy carrier for use in transportation systems and can aid in leveling the power output from renewable power plants.
- A promising technology for generation of renewable H_2 is concentrated solar water splitting, whereby thermally reduced metal oxides are used to split H_2 from steam at high temperatures.
- The economic competitiveness of this type of system needs to be established through rigorous technoeconomic analysis, which can only be accurately performed once operational data are available from prototypical systems.
- Akash developed a simple user interface panel for data acquisition and to virtually control reactor components in a prototype of a solar water splitting system. In addition, he linked the complex process data stream to software with options for various sensor fusion visualization models.

Eliminating Soot Production in Diesel Engines
SULI participant from Sandia National Laboratories (SNL)



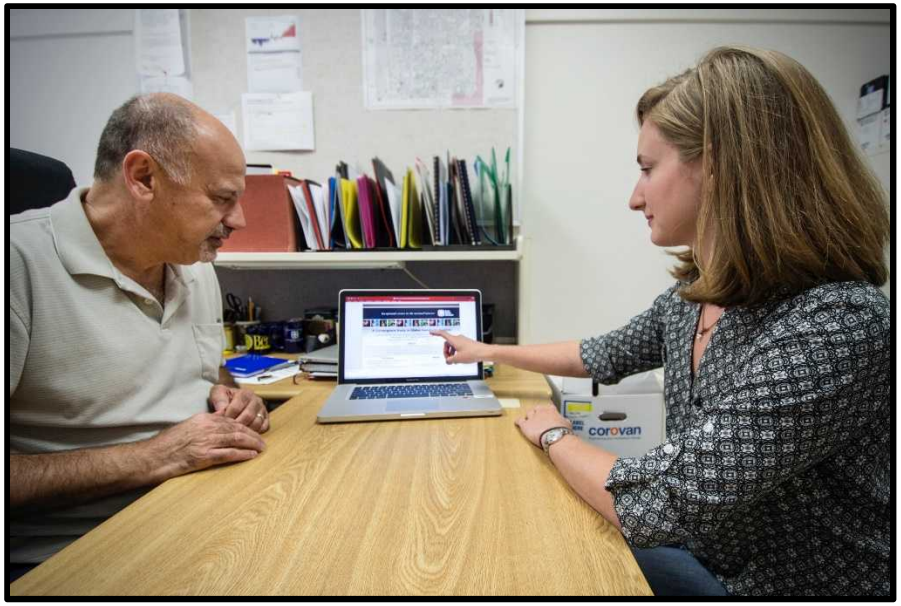
Mr. Daniel Ruth (right), a senior from Penn State University, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"I enjoyed working with leading researchers to analyze data from high-tech cameras and help develop a technology that could have an important societal impact."

- Researchers at Sandia National Laboratories have discovered a novel way to eliminate soot production in diesel engines – using ducted fuel injection (DFI). DFI enhances the mixing between the injected fuel spray and the surrounding air in the engine cylinder, making the fuel-air mixture leaner and dramatically reducing soot formation.
- Daniel developed data analysis tools to process and display the results from an extensive experimental database including over 60 distinct experiments with 10 data streams (including 5 high-speed cameras) and variation of 8 different parameters.
- In particular, Daniel developed an improved methodology for identifying and tracking the location of the tip of the fuel spray.
- Daniel also developed a data screening tool that allows one to search and display results from experiments meeting a chosen set of criteria.

Global Sensitivity Analysis of Chemical Reaction Models

SULI participant from Sandia National Laboratories (SNL)



Ms. Rebecca Harmon (right), a junior from Iowa State University, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"I really enjoyed all of the learning opportunities that were available to me as an intern at a national laboratory. I am going to let others know how positive this experience was for me and I aspire to be employed at a national lab in the future."

- Global sensitivity analysis (GSA) is used to assess the sensitivity of model predictions to the combined effects of uncertainty in the model inputs. For large model systems, as are often used to describe series of chemical reactions, Monte Carlo (MC) sampling is typically used to determine the GSA.
- Rebecca investigated the dependence of Sobol sensitivity indices, a variant of MC sampling-based sensitivity, that measures the fraction of the total variance in the output of a model attributable to one or more individual parameters.
- Rebecca's work demonstrated that the calculated Sobol indices converge (i.e. their error decreases) as the number of samples increases, according to a $N^{-1/2}$ relationship.

Understanding Soot Emissions from Diesel Engines

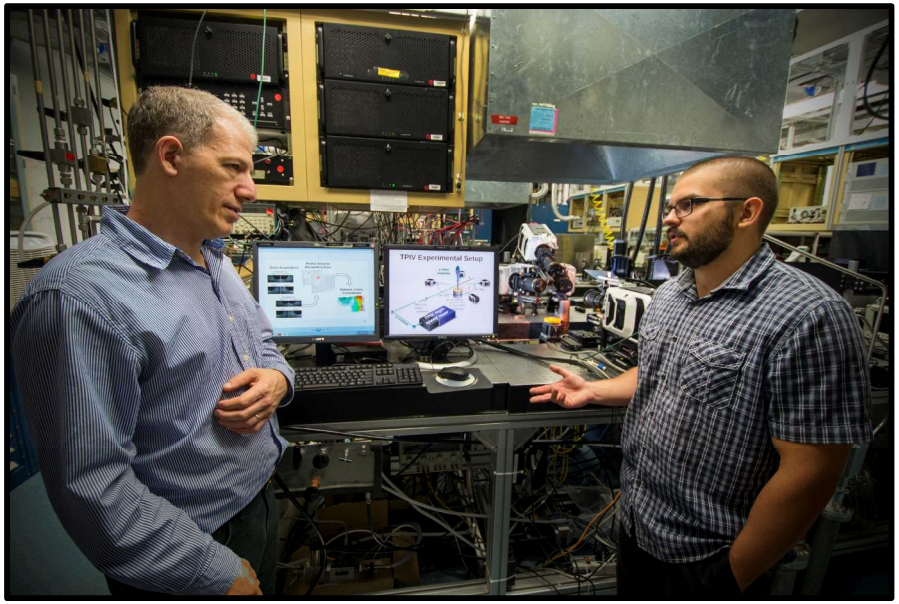
SULI participant from Sandia National Laboratories (SNL)

Mr. Ian Liu (right), a junior from UC San Diego, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"It is very exciting to be studying the details of reactions and mixing that occur inside engines and to relate that to something as practical as soot emissions out the tailpipe."

- The need to meet current stringent emission regulations for soot strongly constrains the design of diesel engines and limits opportunities for efficiency improvements.
- To investigate the relationship between soot formation during the fuel combustion process inside a diesel engine cylinder and the amount of soot actually emitted from the engine, Ian calculated the spatially and temporally integrated soot luminosity signals and compared them against engine-out soot emission for a variety of different engine operating conditions.
- Ian found that for some conditions that amount of soot formed during combustion was actually inversely correlated with the amount of soot emitted, presumably due to the strong role of oxidation on the net amount of soot emitted.

Lagrangian Particle Tracking in Turbulent Flows
SULI participant from Sandia National Laboratories (SNL)



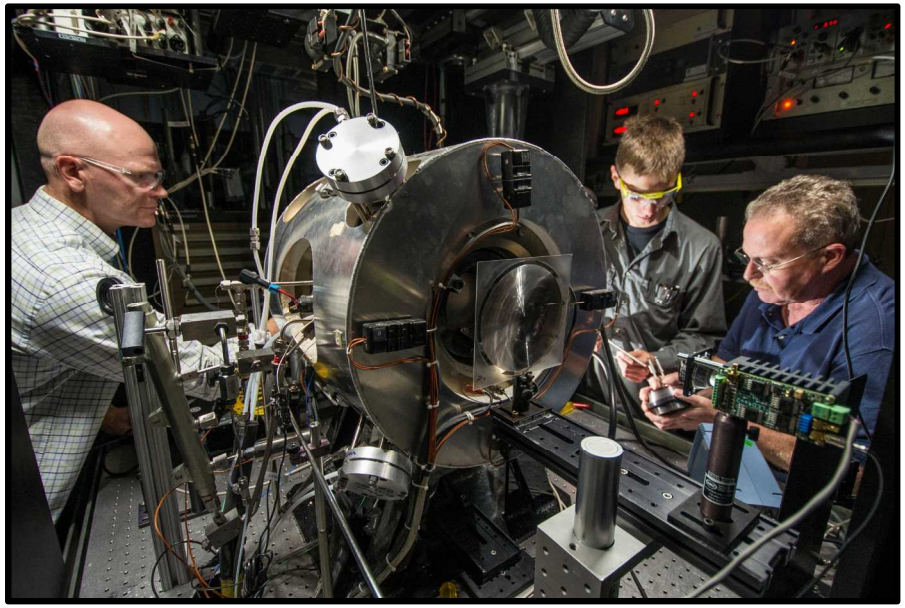
Mr. Maksym Zhelyeznyakov (right), a senior from Texas Tech University, participated in the SULI 2016 Summer Term at Sandia National Laboratories.

"The amount of information that can be generated from modern scientific camera systems is amazing. I was glad to help determine what part of the data you could trust, and what is still a little questionable."

- Turbulent flows occur in the atmosphere and in engines – anywhere that there is rapid mixing. Turbulence can be characterized using Eulerian statistics (wherein the viewer remains in a fixed position) or Lagrangian statistics (wherein the viewer moves with the local flow in space and time).
- Max implemented a Lagrangian particle tracking tool that was used to interrogate a perfectly accurate 3-dimensional direct numerical simulation (DNS) of turbulence from Johns Hopkins University. By adjusting the grid resolution from the DNS results, the influence of the spatial resolution of velocity measurements on the accuracy of derived Lagrangian quantities was determined.
- The results of Max's analysis showed that experimental 3-D high-speed tomographic particle image velocimetry (PIV) data collected in flames has small inaccuracies in velocity, but that the derived vorticity field can have significant biases.

Designing Optical Components for Spray Combustion Experiments

CCI participant from Sandia National Laboratories (SNL)



Mr. Aaron Czeszynski (middle), a second year student at Las Positas JC, participated in the CCI 2016 Summer Term at Sandia National Laboratories.

"I enjoyed working with my hands and my mind to come up with unique solutions to challenging hardware problems."

- Advanced analysis of how high-pressure jets of liquid fuel breaks into small droplets that then evaporate and burn requires custom-designed hardware to mount windows, optical detectors, fiber optics, etc.
- Aaron worked closely with technicians and research staff to design, machine, and install various components that will be part of a new, continuous flow spray combustion experiment.