Christopher Hayes

Class of 2019

Computer Science

Building Open-Source Software to Better Understand the Impact of Soot on Global Warming

Mentors: Professor Chong Qiu, Professor Frank Breitinger

This project began with a need for an improved fractal modeler of atmospheric soot. An available fractal modeler called FracMAP does not account for the overlap of soot nanospheres. Soot nanospheres will overlap to form a group of nanospheres called an agglomerate as a result of sintering. A study on the effects of black carbon nanosphere overlap on the absorption and reflection of light found this effect to be non-trivial (Exposito, 2015, 141-154). This SURF project was focused on integrating this overlap into the FracMAP fractal creation algorithm. To make the application more widely available and readily configurable for researchers, the graphics library was switched from wxWidgets to libigl. Any user who is acquainted with MATLAB will find Libigl's core functions to be similar. FracMAP's command line parser was rewritten to allow a greater level customizability including multiple runs, extended logging, and control over the algorithm's precision. At the start of the project we were planning to also analyze the results of a light simulation on the soot agglomerate model. As the project progressed we realized that goal may be too broad so we updated the scope of the project to focus on building an accurate model of a soot agglomerate.

This research project was generally pretty straightforward, we did not encounter any major surprises or obstacles throughout the project. Implementing our solution involved introducing a variable, k, to control overlap and adjusting the fractal algorithm to accept this new parameter. We had not completed exhaustive testing of the current algorithm to determine whether the fractals generated match experimental data. The monte-carlo algorithm used will generate a random fractal and when we compare a large batch of runs to experimental soot shape data we expect the data to be similar. We also plan to run light simulations using ADDA (Amsterdam Discrete Dipole Approximation) on the models that FracMAP generates. If we combine the capability of FracMAP to generate batches of fractal models from input parameters with the light simulation capabilities of ADDA, the results may be able to help explain what kind of impact atmospheric soot has on the greenhouse effect. The original FracMAP code is available on GitHub.com under the GPL license (GNU General Public License). The forked code from this project will also be available on GitHub.com under the same license. We can't wait to see other researchers take advantage of the program's capabilities and expand them further.

Exposito J. J. Lapuerta, M. and F. J. Martos. Effect of Sintering on the Fractal Prefactor of Agglomerates. *Powder Technology, 271:141–154, February 2015.*

Garro M. A. Chancellor S. Herald C. Moosmuller H. Chakrabarty, R. K. Fracmap: A user-interactive package for performing simulation and orientation-specific morphology analysis of fractal-like solid nano-agglomerates. *Computer Physics Communications, 180:1376–1381, August 2009.*