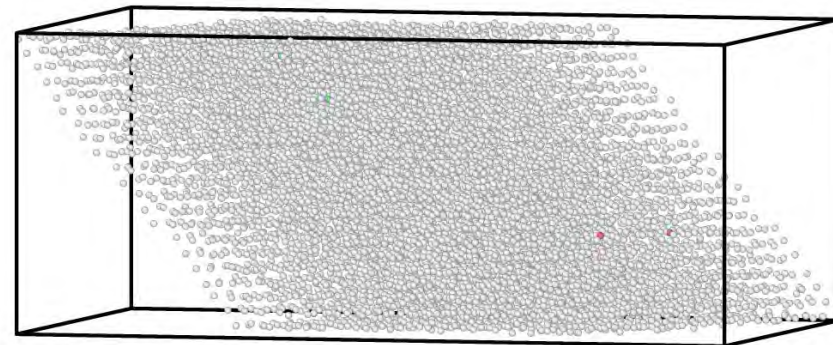
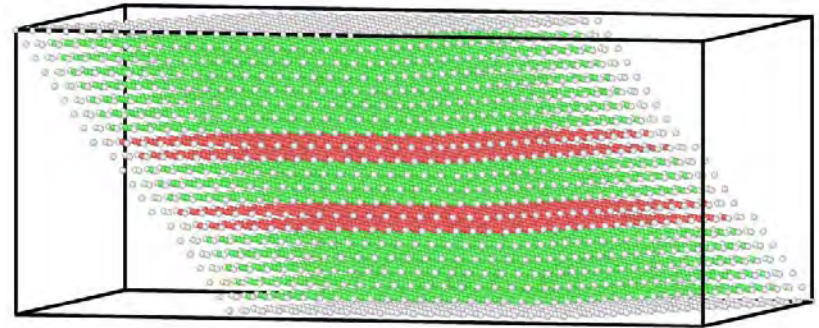


Identifying crystal particle structures and modifying with noise to identify fluctuations

Hunter Shepard¹, Will Wang², Frans A. Spaepen²

¹Southern University and A&M College, ²Harvard University
National Science Foundation, MRSEC, HRD-1736136

The purpose of this project is to improve crystal identification and identify structures from experimental data in colloidal science. Colloidal processes are essential in a variety of industries, including food, pharmaceuticals, pesticides, cosmetics and polymers, and serve as the basis for a wide range of products. The industrial crystallization process is of great interest to the nucleation of crystals from solution, especially when the shape of the crystals is important to their applicability. However, experimental data have thermal fluctuations. Computational Noise is a simulation of naturally occurring error or discontinuity with experimental data. By coding in Python, building three different structures, and adding noise using three different methods, different datasets and visualizations have been developed to display the output data from simulations with Particles and used to investigate. The system is placed on the grid by modeling and computer analysis. The results can be contrasted with experimental results and can provide better insight into the key process variables needed to design a particular shape in a particular crystallization process.



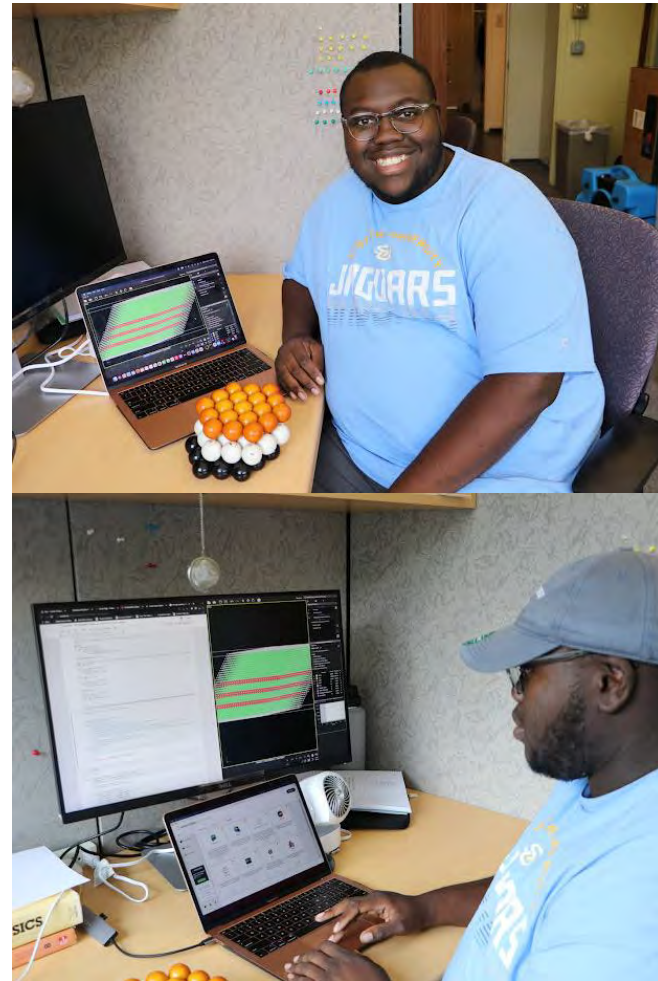
Top: Stacking Fault with no noise . Green=FCC
Bottom: Stacking Fault with 10% noise. Red=HCP

Identifying crystal particle structures and modifying with noise to identify fluctuations

Hunter Shepard¹, Will Wang², Frans A. Spaepen²

¹Southern University and A&M College, ²Harvard University
National Science Foundation, MRSEC, HRD-1736136

Hunter Shepard is a Senior majoring in Mathematics at Southern University and A&M College. During this summer he worked at Harvard University SEAS Applied physics department, Weitz laboratory. In the Weitz lab we research the physics of soft condensed matter, which consists of substances that are easily distorted by forces from the outside, magnetic or electric fields, or even temperature changes. He constructed simulations, writing code, and comparing data analyses. A big challenge for him was learning how to code, and get use to an academic environment within another STEM field. Hunter has done research in Mathematics, biology, chemical engineering, quantum computing, education, but never in applied physics. During the research experience he broadened his research areas and expanded on his knowledge in physics, through this he learned about different crystal structures, colloidal science, and nanoscale materials.



Top: Rendering of Hunter working in office.
Bottom: Photo of code and Ovito simulation.