This past summer, junior Wheaton student Chesterton Schuchardt completed an internship as a research assistant to David Hsu, assistant professor of engineering and physics at Wheaton College. Schuchardt spent several months conducting computational research on shape-memory polymers, which “are a type of dynamic, smart material that have the ability to transform from one shape into another shape when you apply heat to them.” He worked specifically with a polymer called polyethylene, a special plastic that is activated by heat.

Polymers are made up of many molecular chains which, at room temperature, are aligned with one another, which makes it difficult to break the bonds between them. But as the polymer heats up, the increase in energy generates molecular movement. At some point, the chains untangle and are no longer aligned. “If you heat up a [normal] plastic, [the heat] breaks the crystals [the primary molecular bonds] and they flow into equilibrium,” Schuchardt explained. “When you cool it down, it stays in that state and that’s it. But in shape-memory polymers, there are other bonds between chains. These extra bonds work so that when you heat [the polymer], even though the crystals break, there are still permanent net points pulling on the material, trying to get back to the shape it was before. [The crystals] flow into a new shape as it cools down, but when you heat it back up, it’s like there are rubber bands pulling it back to its original shape.”

Since there has already been extensive experimental research conducted on shape-memory polymers, Schuchardt’s work centered around a computational 3D editing software called LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). In this system, he modeled individual molecules in the shape of a cube with side-lengths of 60 nanometers and wrote coding for various simulations such as heat, shape and tension changes. This information was then sent to the supercomputer in Blanchard Hall, which processed these simulations. “Sometimes it takes up to three days to render the simulation, and the amount of data [the supercomputer] receives is only a few nanoseconds. There’s so much math behind it that it takes even a computer that has 512 cores [units that receive and process information — most simple computers only have one or two cores] three days to calculate a nanosecond of data,” Schuchardt described with awe. Once these simulations were complete, he had to analyze the collected data in an attempt to quantify how crystallized the shape-memory polymers were.

Schuchardt shared how “the overall goal of the summer was to develop a relationship between the cross-link density (how many extra bonds there are between individual chains) and how the crystals formed” to contribute to tailoring “a shape-memory polymer for a specific application by understanding how the cross-links affect how [the polymer] melts and how it behaves.” One pivotal application of shape-memory polymers is its contribution to improving human health. Until recently, collapsed arteries needed careful surgical procedures. Now with shape-memory polymers, a very thin, shape-memory tube can be inserted into the artery. As soon as it comes into contact with the patient’s body heat, the tube expands to fill the artery, unblocking that capillary.

There are also fun and practical applications for shape-memory polymers. Schuchardt shared how one team of researchers designed a self-assembling box. Others are looking into a cube the size of a biscuit that, when heated, can self-assemble into a model of the Eiffel Tower. There are huge applications for the storage industry as well, for storing things compactly and only heating them up when they’re needed.

Polymer engineering is an incredible tool that continues to grow and change the way we solve problems. As the research continues to improve and unfold, new applications will arise and provide us with new perspectives. In the words of Schuchardt, “The sky’s the limit.”