**WHY BLUE WATERS**

Blue Waters has allowed us to perform simulations of heat transfer in liquid-solid flow with high resolution that is necessary to capture the correct physics. Capturing the thermal boundary layer is critical for fluid-solid flow since the quantification of fluid-solid heat transfer depends on local temperature gradients across the particle surface. Simulation of heat transfer in liquid-solid flow is time-consuming and costly. The case, as shown in Figure 1, requires 1,200 grid nodes to solve for velocity and temperature fields at a grid resolution of 80. To satisfy the requirements above, Blue Waters is an essential tool for our research to simulate the physics accurately.

**INTRODUCTION**

This research studies the structure of polymers on the microscopic scale. The particular class of polymers are semi-flexible diblock co-polymers (block co-polymers with two distinct blocks) contains polymers useful in flexible electronics, biomedical application, and nano-scale templating. Critical to all of these uses is an understanding of how to control the structures on a nanoscale level. Computational simulations are an efficient way to characterize the structures and explore the polymer compositions that lead to them. Until very recently the computational resources to study semi-flexible polymers did not exist. Now, through the power of the Blue Waters system, it is possible to study these polymers and apply the knowledge of how the structures form to materials design.

**METHODS & RESULTS**

This work has been performed by modeling microparticles of polymers and generating structures in them using a self-consistent field approach that searches for the minimum energy structure with a finite-element method. A broad sweep of polymer properties has identified several candidate structures and work is underway to refine them to create a phase diagram of the structures that form from a given set of conditions. The value of the phase diagram is in its ability to predict the results arising from a given combination of polymer properties. A scientist wishing to generate a particular structure can utilize a phase diagram to design the polymer chains to obtain the final microstructure. Since it is typically possible to control the chain composition to a high degree, the properties required from the phase diagram can be created in an experimental setting. This allows these phase diagrams to be readily applied in experiments.

**CONFINEMENT AND ORIENTATION EFFECTS IN SEMI-Flexible POLYMER STRUCTURES**

**Allocators:** GLCPC/448 Knh

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**EXECUTIVE SUMMARY**

Polymers chains composed of multiple components have the ability to self-assemble into fascinating microscropic structures. The structures they form are reproducible, highly regular, and can be controlled by manipulating the composition of the polymer chains. The chains themselves can range from highly flexible, to extremely rigid. Between these extremes, the class of semi-flexible diblock co-polymers (block co-polymers with two distinct blocks) contains polymers useful in flexible electronics, biomedical application, and nano-scale templating. Critical to all of these uses is an understanding of how to control the structures on a nanoscale level. Computational simulations are an efficient way to characterize the structures and explore the polymer compositions that lead to them. Until very recently the computational resources to study semi-flexible polymers did not exist. Now, through the power of the Blue Waters system, it is possible to study these polymers and apply the knowledge of how the structures form to materials design.

**PUBLICATIONS AND DATA SETS**
