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 gradient along the particle surface. Simulation of heat transfer in liquid-solid flow is time-consuming and costly. The case, as shown in Figure 1, requires $1{,}200^3$ 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.

NEXT GENERATION WORK

We would like to perform PR-DNS simulation of a fluidized bed with a million particles on Blue Waters (using more than 5,000 central processing units) and expect fast data transfer from Blue Waters to local clusters. The goal is to understand instabilities and clustering formation in gas-solid flows, verifying scale separation in the particle phase and provide the ensemble of realizations for small-scale PR-DNS that is used for parametric studies.

PUBLICATIONS AND DATA SETS

Sun, B., Modeling Heat and Mass Transfer in Reacting Gas-solid Flow Using Particle-resolved Direct Numerical Simulation. Ph.D. thesis, Iowa State University, 2016.

CONFINEMENT AND ORIENTATION EFFECTS IN SEMI-FLEXIBLE POLYMER STRUCTURES

Allocation: GLCPC/448 Knh
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EXECUTIVE SUMMARY

Polymer chains composed of multiple components have the ability to self-assemble into fascinating microscopic 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.

INTRODUCTION

This research studies the structure of polymers on the microscopic scale. The particular class of polymers are semi-flexible diblock co-polymers which are a mixture of two components, potentially with vastly different properties. There is great interest in these types of polymers because the mixture of properties enables the resulting material to exhibit behavior desirable in industrial applications, including organic electronics [1], lithographic templating [2], self-assembly [3], and many others.

As the long polymer chains interact with each other, they self-assemble into a wide range of microscopic structures. These structures affect the properties of the resulting material. By combining polymer blocks with differing properties, bulk and surface behavior can be tuned by manipulating the way the polymers organize. As an extension of this, the structures themselves can also be used in building microscopic devices or can be used as a template to control placement of particles in a regular pattern.

Being able to predict and control how polymers organize enables construction of devices that meet specified design goals. If, for example, an application requires a microparticle that exhibits a specific property at regularly spaced intervals along its surface, this can be achieved by selecting one of the polymer components to have that property and then designing the diblock polymer to form a structure that places that polymer at the desired spacing along the surface. This work enables control by determining what structures can be formed and understanding the conditions that are necessary to form them.

Past work has focused predominantly on bulk melts or surface coatings. With the strong interest in nanoparticles and nanostructures, this work uses an alternate calculation method to work with arbitrarily shaped particles to study the structures that form from polymers in nanoparticles. In addition to the ability to model arbitrary shapes, a key aspect of this work is that it utilizes a method to study chains of varying flexibility. **Cutting-edge** polymer applications including, for example, flexible organics often use polymer chains described as semi-flexible. The model used in this work is tailored to these types of chains and can accurately capture the physics they exhibit. While the model itself [4] is not new, the computational power required to use it has prevented the application of it for all but the most basic systems [5]. The power of the Blue Waters system allows this work to focus on a class of polymers and applications that have not been well studied in past simulations.

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.

WHY BLUE WATERS

This research requires a mixture of numerous smaller simulations requiring only a few dozen computational nodes to develop candidate microstructures and several jobs requiring thousands of nodes to refine them. The Blue Waters system provides the high processing throughput to run the smaller jobs in sufficient number to generate the required candidates. It also provides the computational power needed to efficiently run simulations requiring thousands of nodes. Beyond raw computational power, the balance of high system memory, fast inter-process communication, and **high-performance** disk I/O provided the capability to minimize scaling bottlenecks that often arise with calculations on hundreds of thousands of cores. The Blue Waters staff was responsive to requests. They were able to supply information on future software capabilities that was helpful in the development process.

NEXT GENERATION WORK

On a next-generation Track-1 system, this work could be expanded to enable finer resolution of micro-structures. This could allow identification of smaller scale features. Improvements in the simulation software's design to exploit next-generation computational architecture provides an exciting opportunity to **improve efficiency**.

PUBLICATIONS AND DATA SETS

Ackerman, D., and B. Ganapathysubramanian. Parallel framework for wormlike chains using self consistent field theory. *ASME 2015 Applied Mechanics and Materials Conference*, Seattle, WA. July 1, 2015.