treatment of the spin-orbit effect is a reasonable approximation. These results are critically important for development of a comprehensive first-principles approach.

WHY BLUE WATERS

The solution of the Bethe-Salpeter equation is computationally challenging, as it requires computing very large exciton Hamiltonian matrices (ranks more than 100,000). We use either an iterative diagonalization scheme to compute their eigenvalues, or we employ a time-propagation approach to compute optical absorption spectra. Each run requires large amounts of memory, disk storage, and fast communication between the two. Many calculations are needed to ensure convergence of spectra and exciton binding energies on Brillouin zone sampling. Blue Waters provides an outstanding computational package that allows us to carry out these simulations for complicated materials such as CH3NH3PbI3.

Interactions with the Blue Waters team were extraordinarily helpful. As a result, we are now involved in the Joint Laboratory for Extreme Scale Computing (created as part of the Blue Waters Project) aimed at using the efficient ChASE iterative diagonalization scheme to compute their eigenvalues, which fully account for free-carrier screening and electron-phonon effects such as lattice screening, with mesoscale simulations. Furthermore, large-scale materials design requires a large number of such accurate calculations, which, due to their extreme computational cost, can only be achieved on a future Track-1 system. Finally, extending this work towards nanoscale materials such as semiconductor nanocrystals or nanoplatelets will push the computational capabilities of current supercomputers, requires the availability of a future Track-1 system to be successful.

This material is based upon work supported by the National Science Foundation under Grant No. CBET-1437230.

INTRODUCTION

An improved understanding of fluid-solid heat transfer is crucial for process and component design in multiple engineering applications such as pneumatic conveying systems that transfer powders, granules, and other dry bulk materials through an enclosed pipeline using a combination of pressure differences and the flow of a gas, such as air or nitrogen. The use of computational fluid dynamics (CFD) simulations of multiphase flow are an efficient alternative to experiments for process and design optimization and are becoming more common. Predictive CFD with accurate sub-models has the potential to improve the efficiency of CO2 capture, as well as clean energy generation technologies. The predictive capability of multiphase CFD simulations depends on models for interphase transfer terms such as the closure model for interphase heat exchange.

Although improved gas-solid heat transfer models for CFD simulations have been proposed [1], they are not verified for liquid-solid heat transfer. Extending these improved models to liquid-solid heat transfer requires high-resolution PR-DNS data that capture the flow and thermal features in the boundary layer surrounding individual particles. Since liquids diffuse momentum faster than heat, the thermal boundary layer in liquid-solid flows is thinner than in gas-solid flows. Therefore, in water-solid flow, higher grid resolution is needed to capture the thermal boundary layer accurately. Resources like Blue Waters are needed to simulate the physics accurately. The outcome of physics-based predictive models of liquid-solid heat transfer will result in the better design of pipelines to transport materials safely and efficiently.

METHODS & RESULTS

To simulate heat transfer in liquid-solid flow accurately, PR-DNS using the Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PURIBM) [2, 3] approach have been performed with high grid resolution. PURIBM solves mass and momentum equations, and the convective-dissipative scalar transport equation in the liquid phase by imposing exact no-slip and no-penetration boundary conditions on the surface of each isothermal particle. The solid phase is represented using an immersed boundary forcing in the computational domain. Figure 1(a) shows contours of non-dimensional fluid temperature in steady flow past a fixed homogeneous bed of 644 monodisperse spheres in the cross-sectional plane of a three dimensional periodic cubic box at solid volume fraction of 0.1, particle Reynolds number of 100 corresponding to water and (b) Prandtl number of 10 corresponding to air. The length of the computational cubic box is (a) 1D and (b) 1.4D, where D is the particle diameter. The flow direction is from left to right. The differences in the shapes of the isotherms between liquid and gas are clearly visible and the benefits of high resolution are also apparent.

EXECUTIVE SUMMARY

Heat transfer between solid particles in a fluid flow occurs in multiple engineering applications, such as pneumatic conveying. The purpose of this work is to simulate fluid-solid heat transfer using particle-resolved, direct numerical simulation (PR-DNS). Gas-solid heat transfer has previously been simulated and modeled using our PR-DNS approach in a steady flow through a fixed bed of spherical particles. To extend these models to account for liquid-solid heat transfer, such as in a flow of sand particles in water, we need higher resolution simulations to capture the thermal boundary layers surrounding individual particles. Blue Waters enables the study of this heat transfer problem in liquid-solid flow regimes. We simulate heat transfer in steady flow past a fixed bed of spherical particles with high resolution. The PR-DNS database allows us to extend the models for gas-solid heat transfer to liquid-solid heat transfer.
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 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.

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 applications, 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 as building microscopic devices or can be used as a template to control placement of particles in a regular pattern.

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 microscopic 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