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 $CH_3NH_3PbI_3$.

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 that also runs on graphics processing units (GPUs). While this is work in progress, the Blue Waters project was instrumental in initiating and facilitating this work.

NEXT GENERATION WORK

A next-generation Track-1 system will be instrumental for advanced computational material science research. In our particular field, the most pressing goal is to connect accurate atomistic studies, 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 that 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.

PARTICLE-RESOLVED DIRECT NUMERICAL SIMULATIONS OF FLUID-SOLID HEAT TRANSFER

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EXECUTIVE SUMMARY

Heat transfer between solid particles in a fluid flow occur 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.

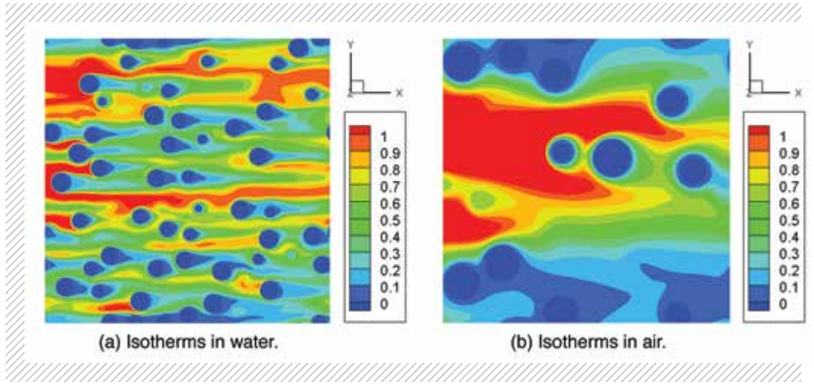

FIGURE 1: A contour plot of the non-dimensional fluid temperature field $\Phi = (T(x,t)-T_s)/(T_{m,in}-T_s)$, where T is the fluid temperature, T_s is the sphere temperature, and $T_{m,in}$ is the bulk fluid temperature, in the cross-sectional plane of a three dimensional periodic computational cubic box at solid volume fraction of 0.1, particle Reynolds number of 20 for (a) Prandtl number of 10 corresponding to water and (b) Prandtl number of 0.7 corresponding to air. The length of the computational cubic box is (a) $15D$ and (b) $7.5D$, 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.

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 differential 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 CO_2 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 (PUReIBM) [2, 3] approach have been performed with high grid resolution. PUReIBM solves mass and momentum equations, and the convective-diffusive 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 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 in a dilute flow (solid volume fraction of 0.1). For this simulation of liquid-solid flow with heat transfer, the grid resolution is $D_m = 80$, where $D_m = D/\Delta x$, D is the sphere diameter and Δx is the grid spacing. The flow direction is from left to right. It is observed that compared with the gas-solid flow in Figure 1(b), the thinner thermal boundary layer forms around each sphere. A thermal wake behind each particle [4] is also seen for the high Prandtl number of 10. Based on these PR-DNS data, extended models for liquid-solid heat transfer are being developed. The extended models for fluid-solid flow will be used in CFD simulations of industrial applications and enable the designer to optimize the design of industrial systems more accurately and efficiently.

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.