DESIGNING MATERIALS IN FLOW: MULTISCALE SIMULATIONS OF COMPLEX FLUID RHEOLOGY

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EXECUTIVE SUMMARY

We developed the first massively parallel, open-source implementation of the multiparticle collision dynamics (MPCD) algorithm for graphics processing units. MPCD is a mesoscale particle-based simulation method for hydrodynamics and is particularly useful for modeling complex fluids and soft matter. Our software will enable studies of complex fluids at length and time scales that would otherwise be inaccessible. We additionally modeled the migration of droplets flowing in microchannels, finding that polymer macromolecules can drive droplets toward the channel center. Such flow-induced focusing of soft materials has important implications for processes ranging from cell sorting to oil recovery.

RESEARCH CHALLENGE

Complex fluids, readily encountered in biology, consumer products, and industrial processing, are multicomponent mixtures that exhibit a rich variety of flow behaviors. A classic example is the cornstarch–water "oobleck" mixture, which acts like a liquid when pressed slowly but can thicken to support the weight of a person when struck quickly. Such peculiar macroscopic flow properties of complex fluids are fundamentally controlled by microscopic molecular structures and interactions. Computer simulations are ideal tools for studying this nontrivial and difficult-to-predict relationship; however, performing simulations of complex fluids at physically relevant scales presents a considerable challenge.

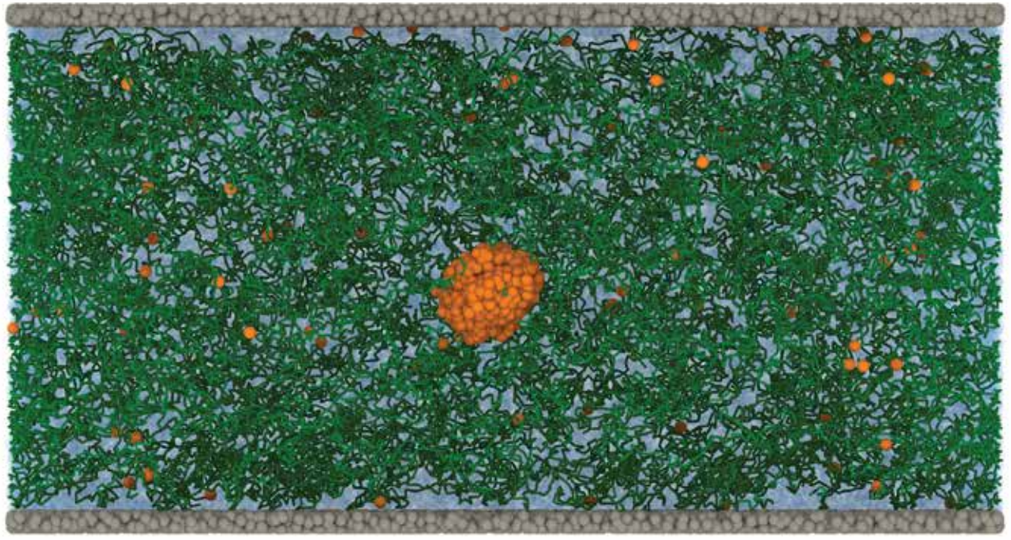

Figure 1: Snapshot of a droplet in a polymer solution under flow simulated using the DPD method. The different DPD particles are: droplet (orange), polymers (green), solvent (blue), and channel walls (grey).

Many complex fluids consist of a mixture of solute macromolecules (polymers) and hard spherical particles (colloids) suspended in a liquid solvent such as water. To obtain the correct dynamics, it is essential to resolve both the direct solute–solute interactions as well as the solvent-mediated interactions. The latter dominates the computational cost for a molecular model of such a mixture; however, a molecular-level description of the solvent itself is often not of interest. A multiscale approach that simplifies the solvent model while preserving its most important interactions is required to study complex fluids at relevant length and time scales.

METHODS & CODES

We applied two particle-based mesoscale simulation methods to simulate complex fluids in flow: multiparticle collision dynamics (MPCD) [1,2] and dissipative particle dynamics (DPD) [3,4]. Both MPCD and DPD significantly accelerate simulations of complex fluids compared to explicit-solvent molecular dynamics models. They employ coarse-grained representations of the solvent that still faithfully reproduce relevant physics such as long-ranged hydrodynamic interactions. However, MPCD and DPD models often still require large numbers of particles with simple interactions, naturally inviting a parallel computational approach. We have leveraged the massive parallelism of graphics processing units (GPUs) with the HOOMD-blue [5–7] simulation package to model complex fluids under flow using MPCD and DPD.

RESULTS & IMPACT

We developed the first massively parallel implementation of MPCD for GPUs, which we released as open-source in HOOMD-blue (version 2.3.0). Flexible initialization and simulation setup are supported through a scriptable Python user interface, while the underlying algorithms have been aggressively optimized to exploit the parallelism of the GPU. Our MPCD software scales efficiently up to 1,024 nodes on Blue Waters. GPU acceleration on the XK nodes exhibited a roughly 3× speedup compared to the XE nodes, which is close to the maximum theoretical performance ratio. The complex fluid and soft matter research communities will significantly benefit from the newly developed MPCD software, which will permit studying processes at physically relevant length and time scales that would be otherwise inaccessible.

We also simulated the migration of droplets in microchannels using DPD (Fig. 1), which is a more mature method than MPCD for modeling multiphase fluids. We found that the addition of polymers to the continuous (solvent) phase induced a migration of the droplets toward the middle of the channel. This flow-induced focusing effect may be exploited during oil recovery to enhance the mobility of oil droplets or used to manipulate soft biological materials such as cells in lab-on-a-chip devices.

WHY BLUE WATERS

Blue Waters is the only system available to us that delivers both the CPU and GPU resources necessary to develop and optimize our MPCD software at scale.

PUBLICATIONS & DATA SETS

Howard, M.P., A.Z. Panagiotopoulos, and A. Nikoubashman, Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration. *Comput. Phys. Commun.*, 230 (2018), DOI:10.1016/j.cpc.2018.04.009.

Michael Howard received a PhD in chemical engineering in May 2018 from Princeton University, where he worked under the supervision of Athanassios Z. Panagiotopoulos.