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–solvent 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 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.

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

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