HAJIM SCHOOL OF ENGINEERING AND APPLIED SCIENCES
UNIVERSITY of ROCHESTER

Department of Chemical Engineering presents

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"Examining the fluid to solid transition of hard polygons with large scale Monte Carlo simulations"

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Two dimensional melting is a fascinating problem that demands powerful simulation tools and compute resources. Hexatic phases with quasi long range bond order and short range positional order require simulations of at least 1 million particles, which take 100's of hours to run on 64 GPUs of the Titan supercomputer. Hard regular polygons approach the behavior of disks for large number of edges, but demonstrate a variety of different melting behaviors for smaller numbers of edges. I will present our results from a study of the melting behavior of regular polygons n=3 to 14. This study would not have been possible without a fast, parallel, and correct simulation code. Our hard particle Monte Carlo implementation performs many trial moves in parallel on a checkerboard grid on the GPU, with a 2nd level of parallelization across multiple MPI ranks, obeying detailed balance. We have implemented overlap checks for a variety of shape classes, including polygons, polyhedra, unions and differences of spheres, and ellipsoids. The discrete element method is another technique to model hard particles with shape, retaining full dynamical information lost in Monte Carlo, but more computationally expensive. These methods will be available open-source in the next release of HOOMD-blue.