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HipGISAXS: A Massively Parallel Code for GISAXS Simulation[1]

SLIM CHOUROU, ABHINAV SARJE, XIAOYE LI, Computational Research Division, Lawrence Berkeley National Lab, ELAINE CHAN, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Lab, HIPGISAXS TEAM — Grazing Incidence Small-Angle Scattering (GISAXS) is a valuable experimental technique in probing nanostructures of relevance to polymer science. New high-performance computing algorithms, codes, and software tools have been implemented to analyze GISAXS images generated at synchrotron light sources. We have developed flexible massively parallel GISAXS simulation software "HipGISAXS" based on the Distorted Wave Born Approximation (DWBA). The software computes the diffraction pattern for any given superposition of custom shapes or morphologies in a user-defined region of the reciprocal space for all possible grazing incidence angles and sample rotations. This flexibility allows a straightforward study of a wide variety of possible polymer topologies and assemblies whether embedded in a thin film or a multilayered structure. Hence, this code enables guided investigations of the morphological and dynamical properties of relevance in various applications. The current parallel code is capable of computing GISAXS images for highly complex structures and with high resolutions and attaining speedups of 200x on a single-node GPU compared to the sequential code. Moreover, the multi-GPU (CPU) code achieved additional 900x (4000x) speedup on 930 GPU (6000 CPU) nodes.

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