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GISAXS simulation and analysis on GPU clusters[1] SLIM CHOUROU, ABHINAV SARJE, XIAOYE LI, Computational Research Division, Lawrence Berkeley National Laboratory, ELAINE CHAN, ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Laboratory — We have implemented a flexible Grazing Incidence Small-Angle Scattering (GISAXS) simulation code based on the Distorted Wave Born Approximation (DWBA) theory that effectively utilizes the parallel processing power provided by the GPUs. This constitutes a handy tool for experimentalists facing a massive flux of data, allowing them to accurately simulate the GISAXS process and analyze the produced data. The software computes the diffraction image for any given superposition of custom shapes or morphologies (e.g. obtained graphically via a discretization scheme) in a user-defined region of k-space (or region of the area detector) for all possible grazing incidence angles and in-plane sample rotations. This flexibility then allows to easily tackle a wide range of possible sample geometries such as nanostructures on top of or embedded in a substrate or a multilayered structure. In cases where the sample displays regions of significant refractive index contrast, an algorithm has been implemented to perform an optimal slicing of the sample along the vertical direction and compute the averaged refractive index profile to be used as the reference geometry of the unperturbed system. Preliminary tests on a single GPU show a speedup of over 200 times compared to the sequential code.

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