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Parallel simulation for block copolymer mesophases MARCO PINNA, XIAOHU GUO, ANDREI ZVELINDOVSKY, University of Central Lancashire, Preston, UK — We develop parallel large-scale Cell Dynamics Simulation to investigate various block copolymer structures. Effective domain decomposition and implementation of boundary conditions gives perfect scaling of the algorithm as function of number of processors. Little simulation time required and large 3 dimensional simulation boxes achievable make the code a good candidate to be a simulation precursor in combination with heavier simulation techniques. We show results obtained for various block copolymer structures, including block copolymer film formation and block copolymer-colloid complexes. Large simulation boxes allow for a realistic account of defects in the systems, which are not effected in such a case by the box size effect. Our method describes time evolution of the systems, and reaches experimental size and time scales.

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