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OpenRBC: Redefining the Frontier of Red Blood Cell Simulations at Protein Resolution[1] YU-HANG TANG, LU LU, HE LI, Brown University, LEOPOLD GRINBERG, VIPIN SACHDEVA, CONSTANTINOS EVANGELINOS, IBM, GEORGE KARNIADAKIS, Brown University — We present a from-scratch development of OpenRBC, a coarse-grained molecular dynamics code, which is capable of performing an unprecedented in silico experiment — simulating an entire mammal red blood cell lipid bilayer and cytoskeleton modeled by 4 million mesoscopic particles — on a single shared memory node. To achieve this, we invented an adaptive spatial searching algorithm to accelerate the computation of short-range pairwise interactions in an extremely sparse 3D space. The algorithm is based on a Voronoi partitioning of the point cloud of coarse-grained particles, and is continuously updated over the course of the simulation. The algorithm enables the construction of a lattice-free cell list, i.e. the key spatial searching data structure in our code, in $O(N)$ time and space space with cells whose position and shape adapts automatically to the local density and curvature. The code implements NUMA/NUCA-aware OpenMP parallelization and achieves perfect scaling with up to hundreds of hardware threads. The code outperforms a legacy solver by more than 8 times in time-to-solution and more than 20 times in problem size, thus providing a new venue for probing the cytomechanics of red blood cells.

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