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High-Efficiency Multiscale Modeling of Cell Deformations in Confined Microenvironments in Microcirculation and Microfluidics HUIJIE LU, ZHANGLI PENG, University of Notre Dame — We developed a high-efficiency multiscale modeling method to predict the stress and deformation of cells during the interactions with their microenvironments in microcirculation and microfluidics, including red blood cells (RBCs) and circulating tumor cells (CTCs). There are more than 1 billion people in the world suffering from RBC diseases. The mechanical properties of RBCs are changed in these diseases due to molecular structure alternations, which is not only important for understanding the disease pathology but also provides an opportunity for diagnostics. On the other hand, the mechanical properties of cancer cells are also altered compared to healthy cells. This can lead to acquired ability to cross the narrow capillary networks and endothelial gaps, which is crucial for metastasis, the leading cause of cancer mortality. Therefore, it is important to predict the deformation and stress of RBCs and CTCs in microcirculations. We develop a high-efficiency multiscale model of cell-fluid interaction. We pass the information from our molecular scale models to the cell scale to study the effect of molecular mutations. Using our high-efficiency boundary element methods of fluids, we will be able to run 3D simulations using a single CPU within several hours, which will enable us to run extensive parametric studies and optimization.

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