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Computational models of the cytoplasm of bacterial cells PETER WILLIAMS, Department of Applied Physics, Yale University, IVAN SUROVTSEV, CHRISTINE JACOBS-WAGNER, Department of Molecular, Cellular, and Developmental Biology, Yale University, MARK SHATTUCK, Benjamin Levish Institute and the Department of Physics, The City College of New York, COREY O'HERN, Departments of Mechanical Engineering Materials Science, Applied Physics, and Physics, Yale University — In vivo experiments of bacteria have shown that free ribosomes and ribosomes bound to mRNA possess dramatically different self diffusion coefficients. In addition, the diffusion coefficient of ribosomes is strongly affected by its interaction with DNA in the nucleoid. We have developed molecular dynamics simulations of mRNA-ribosome complexes (polysomes) in bacteria to investigate the mechanisms responsible for their slow dynamics. In preliminary studies, we showed that polysomes diffuse slower than spheres with an equivalent mass. The introduction of DNA in the simulation gives rise to a further decrease in the diffusion coefficient of polysomes. We quantify the number of entanglements between polysomes to explain the strong decrease in their diffusion coefficient. Static packings of polysomes also indicate that tension in the polysome chain can affect the jamming onset and the packing fraction at which the diffusion coefficient vanishes.

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