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Monte Carlo simulation of single-molecule recycling in a nanochannel for accurate diffusion measurements BO WANG, SULTAN BEHERY, LLOYD M. DAVIS, University of Tennessee Space Institute — In previous experiments on single-molecule (SM) detection in solution, we demonstrated that prolonged observation times and photon yields are achieved by actively trapping a molecule in a nanochannel. We also developed Monte Carlo simulations to optimize experimental parameters and improve real-time control algorithms. Other researchers have since shown similar advantages can be attained by alternating the flow in the nanochannel so that a SM repeatedly passes through the laser excitation focus and that variation in the times between detections provides a measure of the diffusion coefficient of the molecules. We have extended the previous simulations to study the SM recycling experiment and to compare control algorithms and measurement capabilities in which the timing of each photon is processed by an FPGA circuit, as used in our trapping experiments, with those where detected photons are first collected into 1 ms bins, as in the prior recycling experiments. We present capabilities for measuring the diffusion coefficients of SMs. Also, we compare the capability for resolving a solution containing species with differing diffusion coefficients with that of fluorescence correlation spectroscopy, which is often used for monitoring molecular interactions in pharmaceutical research.

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