Millisecond-Long Molecular Dynamics Simulations of Proteins on the Anton Machine

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The ability to perform long, accurate, atomic-level molecular dynamics (MD) simulations could in principle provide insights into the structural, dynamic, and functional characteristics of proteins at an atomic level of detail. Many biologically important phenomena, however, occur over timescales that have thus far fallen far outside the reach of MD technology. We have constructed a specialized, massively parallel machine, called Anton, that is capable of performing all-atom simulations of proteins in an explicitly represented solvent environment at a speed roughly two orders of magnitude beyond that of the previous state of the art. Using novel algorithms developed within our lab, the machine has now simulated the behavior of a number of proteins for periods as long as a millisecond -- approximately 100 times the length of the longest previous MD simulation -- revealing aspects of protein dynamics that were previously inaccessible to both computational and experimental study.