Daniel Standage
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Molecular Dynamics Readings

The first paper provided a brief review of molecular dynamics and how advances in computer technology have enabled the simulation of more complex proteins for longer time periods. By noting that the complexity of MD simulations increases linearly with simulated time and quadratically with the number of simulated atoms, the authors made some projections about when it may be feasible to carry out MD simulations for large biomolecules (of significant biological interest) at a reasonable time scale. What struck me most about this review, however, was the comparison of our current MD simulation capabilities with the MD pioneers. It's hard for me to comprehend the difference between small time scales (second, millisecond) and extremely small time scales (nanosecond, picosecond), and yet the difference is staggering. Comparing a second to millions of years of geological time helped me realize how far we've come and how far we can go with our current trajectory.

The second paper brought up the very important question as to whether reliable biological conclusions can be drawn from MD simulations alone. The paper described the same limitations mentioned in the first paper: biomolecular size and biologically relevant timescales. It then went on to describe how coarse-graining structures and the application of additional forces (steered MD or SMD simulations) can be used to improve simulations, as demonstrated by 3 or 4 use cases.