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Simulating protein folding and aggregation on the 10 second timescale

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Understanding how proteins self-assemble or "fold" is a fundamental problem in biophysics. Moreover, the ability to understand and quantitatively predict folding kinetics would have many implications, especially in the area of diseases related to protein misfolding, such as Alzheimer's Disease. However, there are many challenges to simulating folding, most notably the great computational challenges of simulating protein folding with models with sufficient accuracy to make quantitative predictions of experiments. In my talk, I will discuss our recent work to combine distributed computing with a new theoretical technique (Markov State Models) in order to simulate folding on long timescales as well as the direct and quantitative experimental tests of these methods. I will conclude with the application of these methods to the study of the Abeta peptide, whose aggregation has been directly implicated as the toxic element in Alzheimer's Disease.