

# Computer simulations of biological change

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Computational models have huge potential to provide insight into molecular biology as they are able to take the inherent complexity of these systems into account. Molecular dynamics is an established simulation technique that is widely used to study biomolecular structure, biomolecular dynamics and molecular recognition. However, the expense of the calculations, which require high performance supercomputer facilities, places serious limitations on the length and time-scales that can be accessed. I shall describe the successes and the challenges of simulations of biomolecules using examples from our own research; namely DNA packing and protein aggregation into amyloid fibrils, and will comment on future prospects.

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*Sarah Harris became interested in using theoretical physics to describe biomolecules while studying physics at the University of Oxford. She subsequently obtained a PhD in computational biophysics from the School of Pharmacy in Nottingham in 2001, and then spent three years working as a postdoctoral research assistant at University College London in the area of nonequilibrium computational physics. In 2004 she was appointed as a lecturer in biological physics in the Polymers and Complex Fluids Group in Physics and Astronomy at the University of Leeds. She now has a lively research group working in the area of computational biophysics. She teaches lecture courses in statistical mechanics and computational physics.*