The Computational Microscope Images Biomolecular Machines and Biomedical Nanodevices

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Over the past three decades computational biology has made great strides into simulating biomolecules at ever more relevant time scales and length scales. Today biomolecular assemblies can be followed for many microseconds and at multi-million atom size. The simulations have passed many tests successfully and often offered entirely new views that conventional microscopy could not furnish. In fact, computer simulations take the place of a new type of microscopy, ideally suited for the nanoscale relevant for studies of living cells and for designing new devices in nanotechnology. While being impressive on its own, the computational microscope excels most in conjunction with other types of microscopies, a key example being the combination of X-ray scattering, electron microscopy and computational microscopy. Structures and processes can be visualized over wide spatial (Angstrom to micrometer) and time (picosecond to 10 microsecond) scales. Applications include integral views of proteins exerting forces on cells or sculpting cellular membranes, of ribosomes in different functional states, and of entire (70 nm size including hundreds of proteins) photosynthetic organelles absorbing sun light and charging the cellular membrane. The advanced software and hardware technologies that make the computational microscope feasible will also be outlined.