

MACROMOLECULAR MODELING & BIOINFORMATICS

Theoretical & Computational Biophysics Group at UIUC

The Resource studies living systems that constitute themselves through self-organized aggregation of their molecular components. Research focuses, in particular, on the formation, structure, and function of biopolymer aggregates forming bioenergetic proteins, complexes of membranes with proteins, or complexes of DNA with chromosomal and regulatory proteins. The investigations explore the physical mechanisms underlying the transformation of light energy into electrical membrane potentials and the synthesis of ATP in photosynthetic systems, as well as the mechanical functions of proteins, e.g. in muscle.

The Resource develops software for large-scale simulations. Software tools include NAMD, recipient of a 2002 Gordon Bell Award, a molecular dynamics simulation program used for classical, atomistic molecular dynamics simulations of large biomolecular aggregates; VMD, a molecular visualization program for displaying, animating, and analyzing both large and small biomolecular systems using 3-D graphics and built-in scripting; BioCoRE, a web-based, tool-oriented collaboratory for biomedical research and training.

The Resource has integrated recently its VMD and NAMD software into a comprehensive research tool which permits interactive molecular dynamics with a

haptic (force feedback) interface that allows researchers to manipulate biomolecular model systems in parallel with single molecule experiments, e.g., atomic force microscopy studies.

Ongoing investigations include studies of aquaporin channels, mechanosensitive channels, ATP synthase, a chloride channel, photosynthetic proteins, visual receptors, and proteins with mechanical functions. Development seeks efficient evaluation of force fields and integration schemes for simulation of very large biomolecular systems as well as efficient distributed molecular dynamics programs on workstation clusters and massively parallel machines.

Learn more about the NIH Resource for Macromolecular Modeling and Bioinformatics, visit www.ks.uiuc.edu.

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Image: The image shows a simulated model of a membrane embedded mechanosensitive channel (220,000 atoms), representing large scale biological simulations conducted by the Resource.

