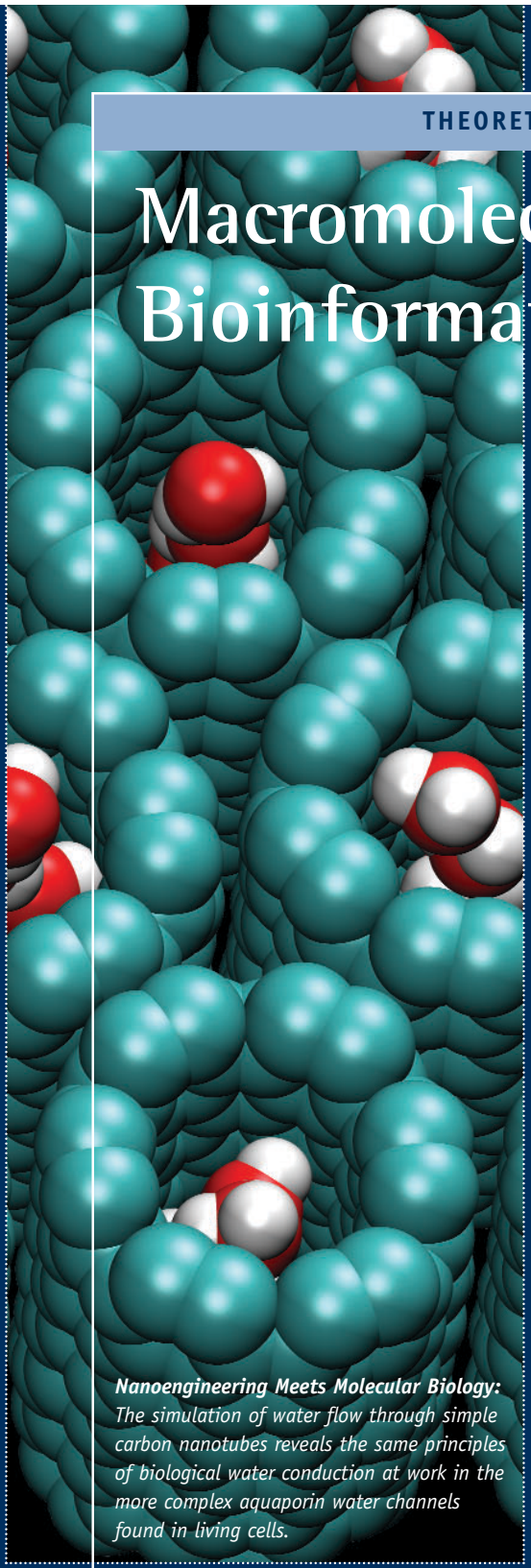
Macromolecular Modeling and Bioinformatics



Nanoengineering Meets Molecular Biology: *The simulation of water flow through simple carbon nanotubes reveals the same principles of biological water conduction at work in the more complex aquaporin water channels found in living cells.*

The resource studies large biomolecular processes in living cells, focusing on membrane proteins that mediate the exchange of materials and information across, in particular, biological membranes as well as the conversion between electro-osmotic, mechanical, and chemical energy. It also develops software for large-scale simulations. Software tools include NAMD, 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.

Interactive molecular dynamics *(IMD)* for the manipulation of molecular simulations with real-time force feedback and interactive display; investigations of aquaporin channels, mechanosensitive channel, ATP synthase, chloride channel, photosynthetic proteins, visual receptors, and proteins with mechanical functions; efficient evaluation of force fields and integration schemes for simulation of very large biomolecular systems; efficient distributed molecular dynamics programs on workstation clusters and massively parallel machines; continued development of NAMD, VMD, and BioCoRE.

NAMD, VMD, and BioCoRE are the three flagship software packages developed by the NIH Resource for Macromolecular Modeling and Bioinformatics at the University of Illinois. NAMD, recipient of a 2002 Gordon Bell Award, is a parallel, object-oriented molecular dynamics code designed for high-performance simulation of large biomolecular systems. VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. BioCoRE is a collaborative work environment for biomedical research, research management and training.

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

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BioCoRE NAMD VMD

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