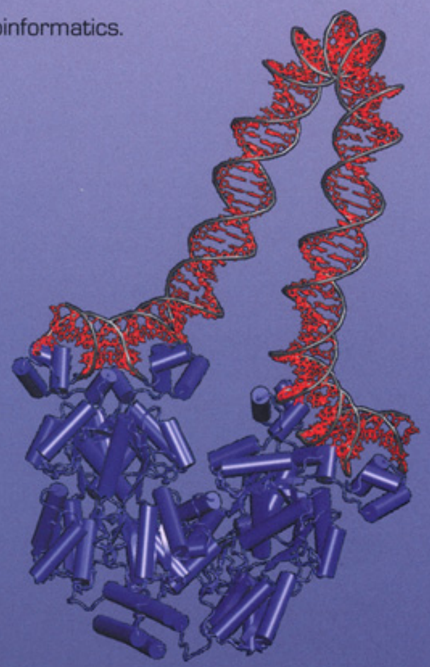
TCBG Theoretical and Computational Biophysics Group

The Theoretical and Computational Biophysics Group brings molecular graphics, molecular modeling, bioinformatics, and collaboration software to bear on questions of biomedical relevance. Research and development activities center on the structure and function of supramolecular systems in the living cell, and on the development of efficient computing tools for the life sciences. Directed by Professor Klaus Schulten, this multidisciplinary group operates the NIH Resource for Macromolecular Modeling and Bioinformatics.



Theoretical and Computational Biophysics Group

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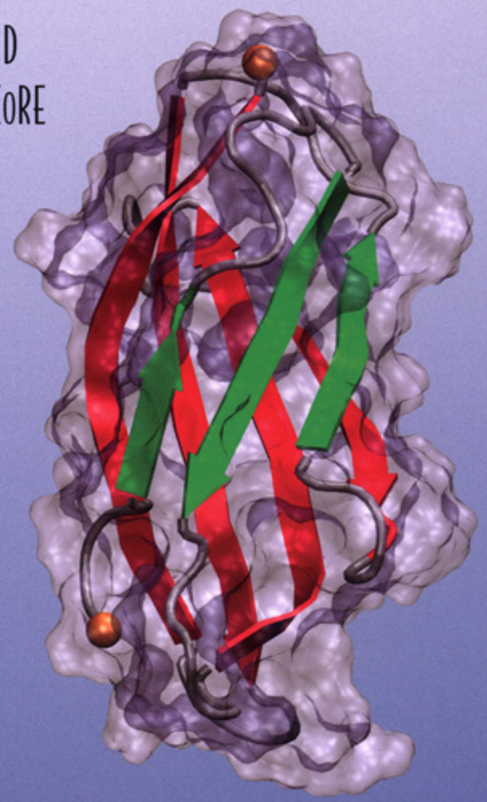
VMD
NAMD
BioCoRE



VMD: http://www.ks.uiuc.edu/Research/vmd/

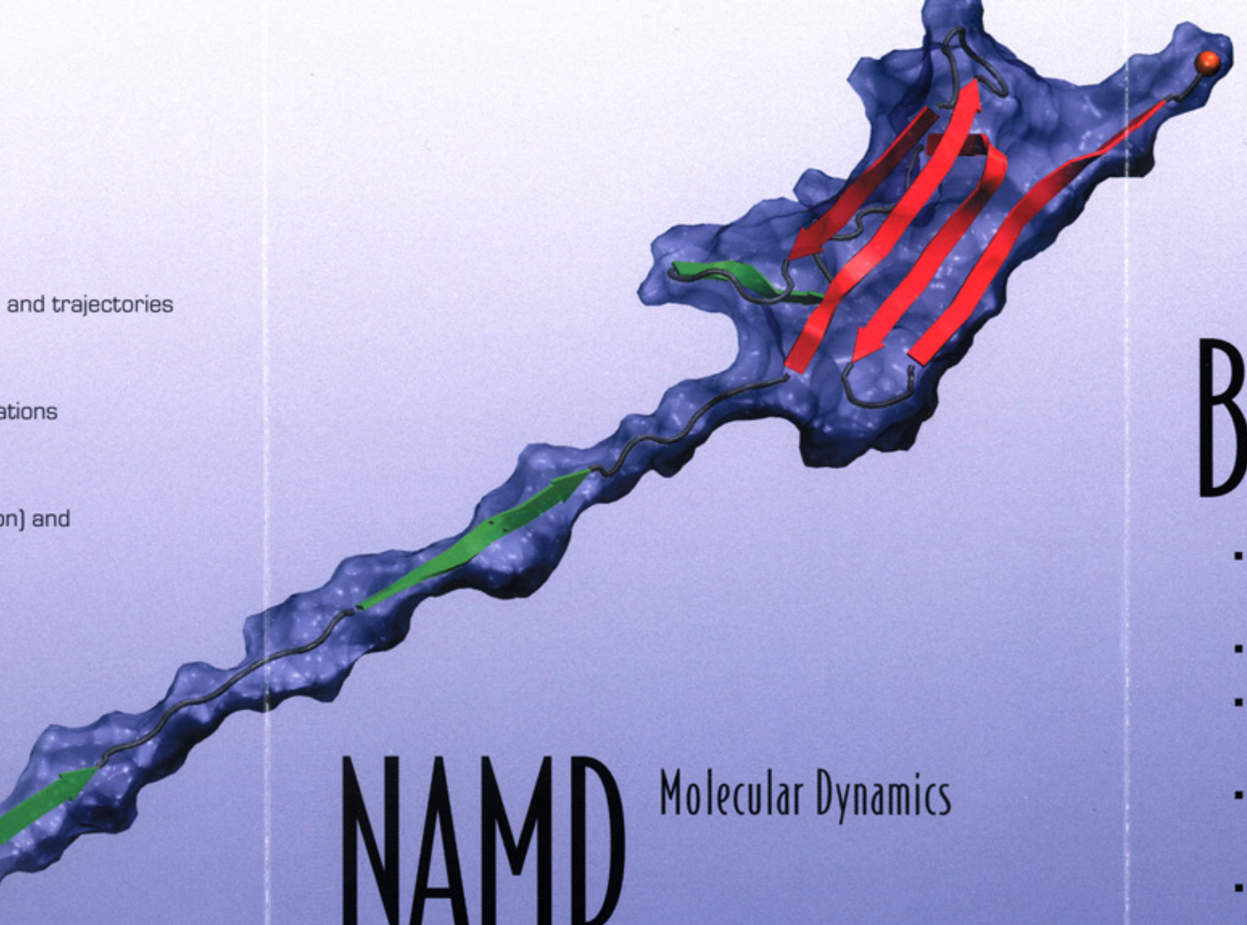
NAMD: http://www.ks.uiuc.edu/Research/namd/

BioCoRE: http://www.ks.uiuc.edu/Research/biocore/

All software is freely available for download.

VMD
Molecular Graphics

- interactively displays sequences, structures, and trajectories
- facilitates structure building and analysis
- drives interactive molecular dynamics simulations
- permits shared visualization sessions
- provides user-extensible scripting (Tcl/Python) and C/C++ plugins
- runs on Mac, Windows, and Unix



NAMD
Molecular Dynamics

- simulates biomolecular systems of thousands to millions of atoms
- works with CHARMM, AMBER, and GROMACS force fields and files
- allows interactive steering through VMD
- runs on most platforms, including Mac and Windows desktops, Linux clusters, and massively parallel supercomputers
- implements full electrostatics, constant pressure and temperature ensembles, free energy perturbation, and several steering methods

BioCoRE
Collaborative Research

- provides a web-based collaborative environment for biomedical research, research management, and training
- organizes group research by projects
- supports co-authoring and sharing of documents through a shared file system
- simplifies supercomputer simulation management using the Grid
- allows sharing of molecular visualization results over the internet
- includes instant messaging, making it easy to communicate in a secure, private environment
- enhances access to VMD and NAMD in a single location
- runs on all major platforms