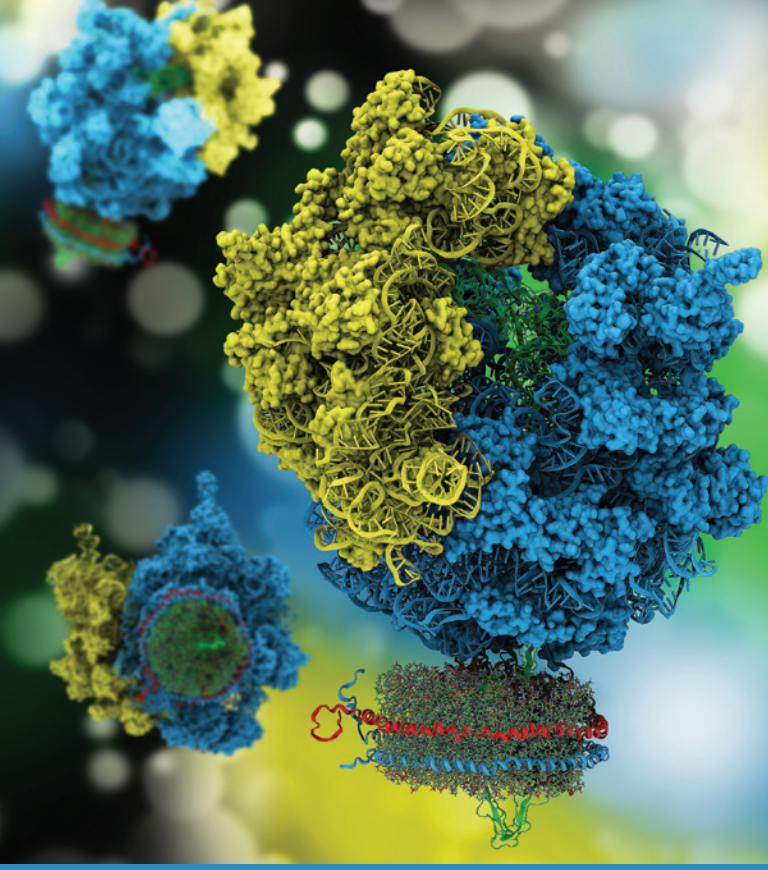

NAMD

Scalable Molecular Dynamics

www.ks.uiuc.edu/Research/namd

NAMD is freely available for download.

ILLINOIS

NAMD

Scalable Molecular Dynamics

- designed for large biomolecular systems
- scales from the laptop to the petascale
- runs on Mac, Windows, and Linux laptops and desktops, Linux clusters, and Cray and IBM supercomputers
- supports NVIDIA CUDA GPU acceleration
- distributed free of charge as source code and convenient precompiled binaries
- integrated with VMD for simulation setup and analysis
- Tcl-based scripting for easy customization
- runs the same input files on any number of processors
- CHARMM and Amber force fields and molecular data files
- explicit water and ions or implicit solvent model
- alchemical free energy calculations
- comprehensive collective variable definitions for free energy calculations, biases, steering, and multidimensional analyses
- scriptable replica system for parallel annealing, Hamiltonian exchange, and umbrella sampling in arbitrar y dimensions
- molecular dynamics flexible fitting to cryo-electron microscopy data via grid-based forces with symmetry and domain restraints

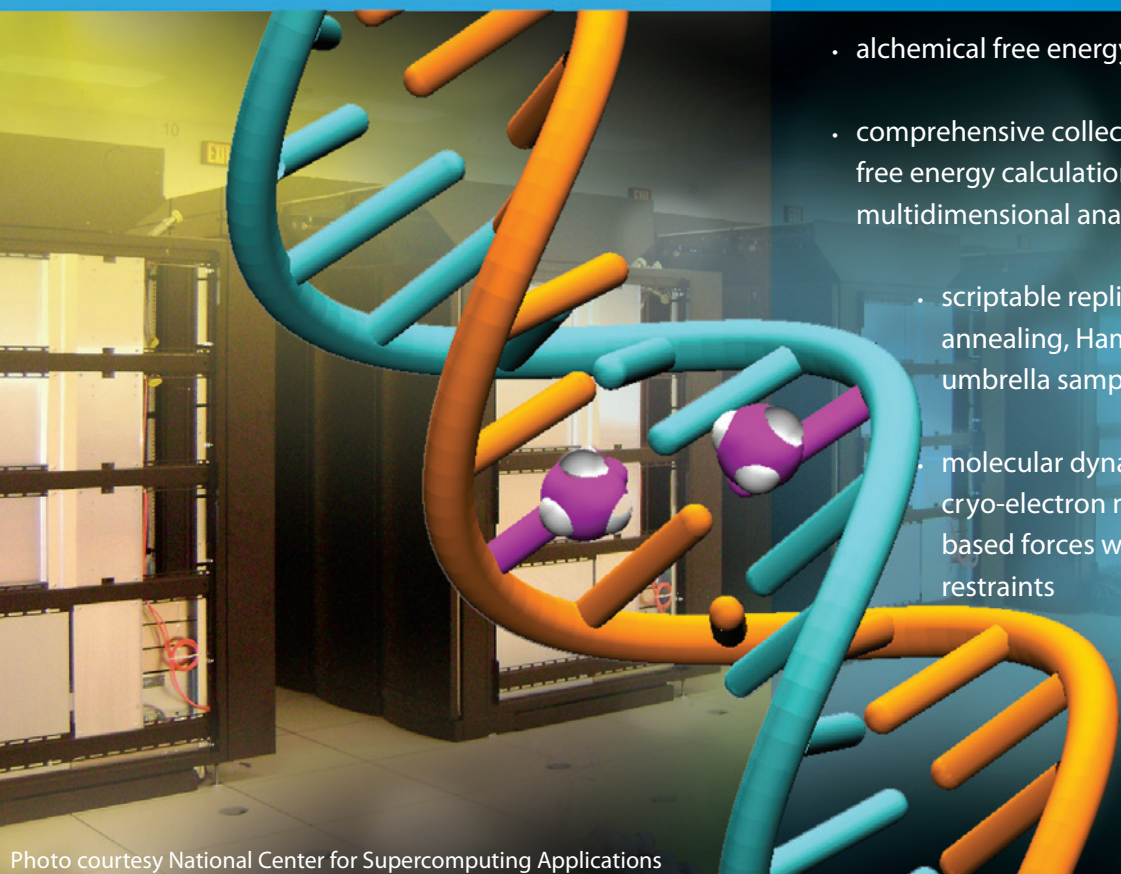

Photo courtesy National Center for Supercomputing Applications

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The Theoretical and Computational Biophysics Group (TCBG) brings molecular graphics, molecular modeling, and bioinformatics software to bear on questions of biomedical relevance. Research and development of 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, the multidisciplinary TCBG operates the National Institutes of Health Biomedical Technology Resource Center for Macromolecular Modeling and Bioinformatics.