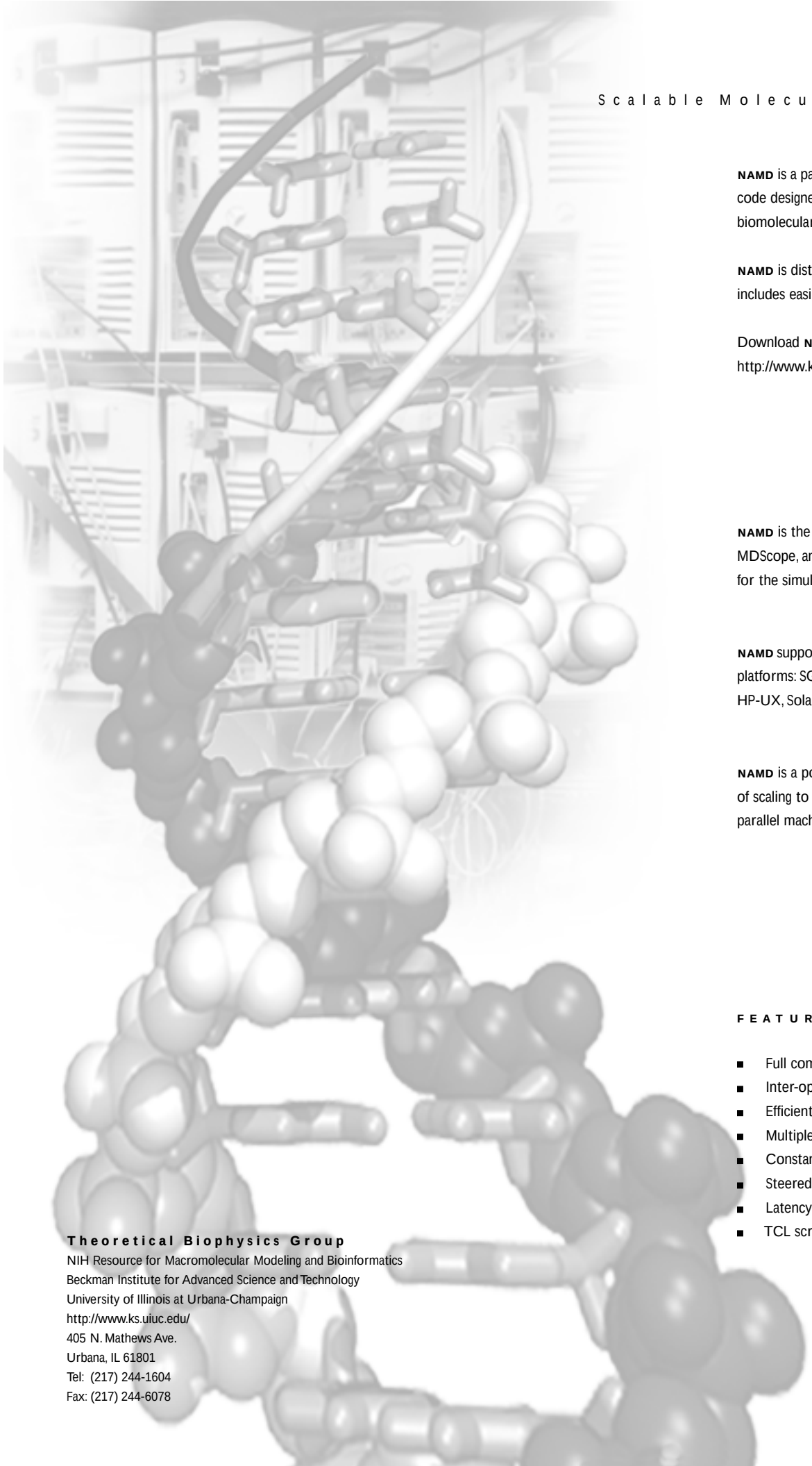

NAMD

Scalable Molecular Dynamics

NAMD is a parallel, object-oriented molecular dynamics code designed for high-performance simulation of large biomolecular systems.

NAMD is distributed free of charge and includes easily modified C++ source code.

Download **NAMD** from
http://www.ks.uiuc.edu/Research/namd/

NAMD is the molecular dynamics component of MDScope, an interactive visual computing environment for the simulation and study of biological aggregates.

NAMD supports a wide variety of computing platforms: SGI Origin 2000, Cray T3E, and HP-UX, Solaris, Alpha and Linux clusters.

NAMD is a powerful computational engine capable of scaling to hundreds of processors on massively parallel machines.

FEATURES

- Full compatibility with the CHARMM force field
- Inter-operability with CHARMM and X-PLOR
- Efficient full electrostatics via Fast Algorithms
- Multiple timestepping and rigid bonds (SHAKE)
- Constant pressure and temperature integration
- Steered Molecular Dynamics (SMD) capabilities
- Latency tolerance for performance on clusters
- TCL scripting language

Theoretical Biophysics Group
NIH Resource for Macromolecular Modeling and Bioinformatics
Beckman Institute for Advanced Science and Technology
University of Illinois at Urbana-Champaign
http://www.ks.uiuc.edu/
405 N. Mathews Ave.
Urbana, IL 61801
Tel: (217) 244-1604
Fax: (217) 244-6078