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MOLECULAR DYNAMICS OF LIPID BILAYERS

DR. MARK NAGUMO
NAVAL RESEARCH LABORATORY
BIO/MOLECULAR ENGINEERING BRANCH
WASHINGTON, DC 20375-5000

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The aim of this work is to study, by molecular dynamics simulations, the properties of model lipid bilayers. We have applied the vectorizable, order-N Monotonic Lagrangian Grid near-neighbors algorithm and have developed a novel constraint algorithm to a simple model bilayer system. We have developed fast angle-dependent force/potential algorithms to treat angle bending and torsion.

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         Naval Research Laboratory
         Washington, DC 20375-5000

Project Objectives:

The objective of this research is to study lipid bilayer models by molecular dynamics simulations. The computer code, which has been developed on the Cray XMP-24 at the Naval Research Laboratory (NRL), is based on the Monotonic Lagrangian Grid (MLG) near neighbors algorithm developed by Boris and Lambrakos of the Laboratory for Computational Physics and Fluid Dynamics at NRL [1,2]. The MLG algorithm had been developed for simulating diatomic systems such as N_2 [3]. A characteristic deeply embedded in the current realization of the MLG algorithm is two-dimensional periodicity. The direction normal to the periodic plane can be bounded by a reflecting wall or it may be free. A constraint algorithm had been developed and tested to maintain a fixed distance between the constitutive atoms of the diatomic molecules.

There were two paramount problems to solve in order to adapt the molecular dynamics codes to simulations of systems of polyatomic molecules such as lipid bilayers. First, it was necessary to generalize the constraint algorithm to the polyatomic case. This work has been described in publication #1, below. Second, it was desirable to develop an efficient method for calculating the intramolecular angle dependent functions for potentials and forces of torsion and angle bending. The angle-dependent force algorithm determines the directions along which forces are to be applied to particles by projection methods, rather than by calculating cross products. The projection code used fewer expensive operations: the angle-bending algorithm is approximately 7 times faster and the torsion algorithm approximately 40% faster than the cross-product based code. This work has been completed, and a manuscript is in preparation for submission to **Siam J. Sci. Stat. Comp.**

A forty picosecond simulation of a butane system has been conducted to test the performance of the constraint and torsion algorithms. The Ryckaert-Bellemans torsional and intermolecular potential (Lennard-Jones with a cross section of 3.92 Å and well depth of 72 K) were used [4]. The energy of the system versus time is shown in figure 1. The initial angular distribution was chosen with a gaussian random distribution about the trans (0°) minimum of the torsional potentials, and the molecules were assigned random center of mass velocities. The total energy is reasonably well conserved; improvements are possible by using a shorter time step or by using multiple time steps to separate rapid and slow degrees of freedom. The development of the distribution of torsion angles towards the equilibrium Boltzmann distribution is shown in figure 2 at 0, 1, 5, 10, 25, and 40 ps.

Simulations of a C_{10} bilayer are underway.

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3. S.G. Lambrakos, J.P. Boris, R.H. Gurguis, M. Page and E.S. Oran, (1988) **J. Chem. Phys. 90**, 4473-4481.

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Publications:

1. "A Constraint Algorithm for Maintaining Rigid Bonds in Molecular Dynamics Simulations of Large Molecules," S.G. Lambrakos, J.P. Boris, E.S. Oran, I. Chandrasekhar and M. Nagumo, NRL Memorandum Report 6174, March 4, 1988.

2. "A Modified Shake Algorithm for Maintaining Rigid Bonds in Molecular Dynamics Simulations of Large Molecules," S.G. Lambrakos, J.P. Boris, E.S. Oran, I. Chandrasekhar and M. Nagumo, **J. Comput. Phys.**, 1989, in press.*

3. "An Algorithm for Calculating Angle-Dependent Forces on Vector Computers" J.H. Dunn, M. Nagumo and S.G. Lambrakos, in preparation.*

*preprint or reprint available on request to MN
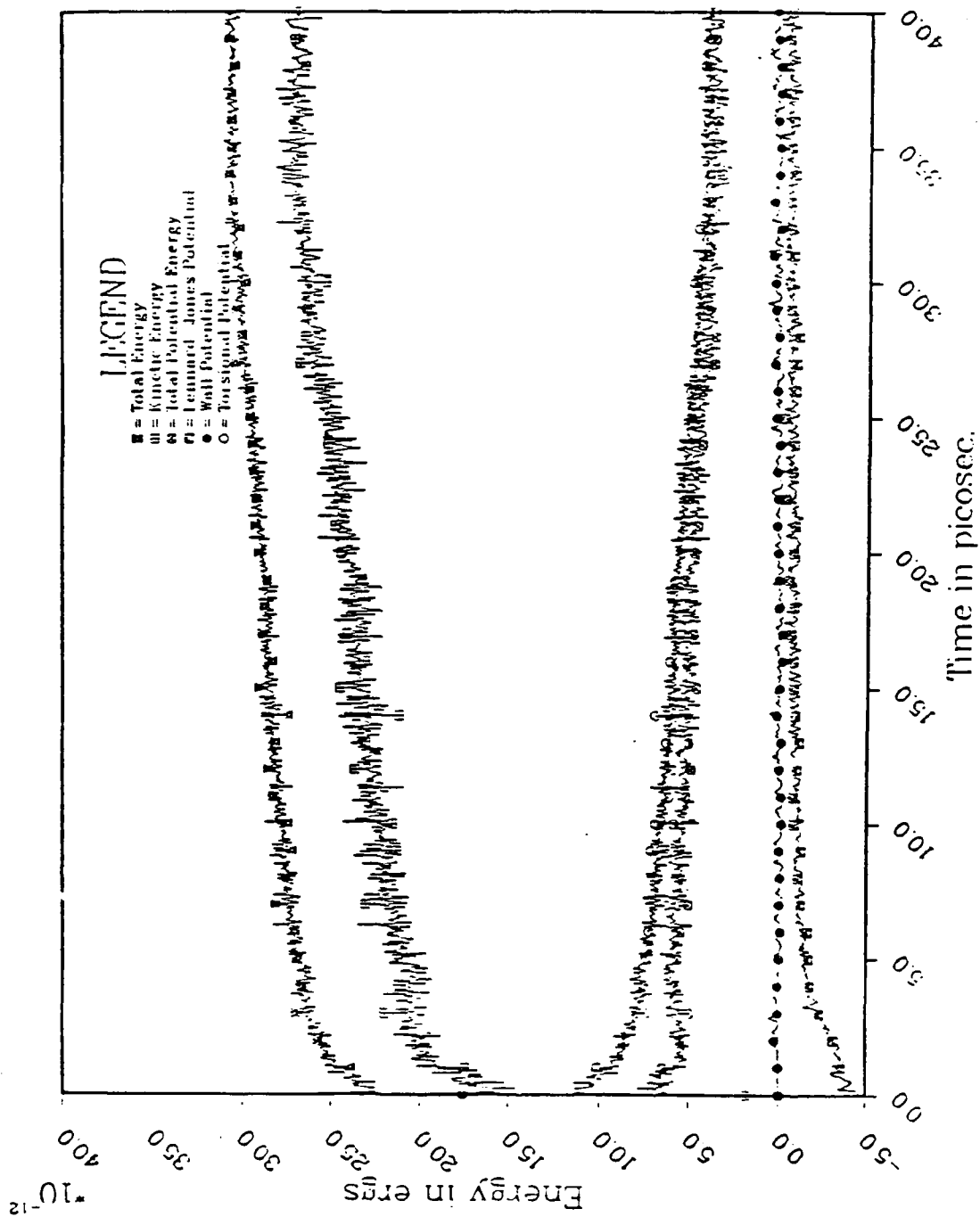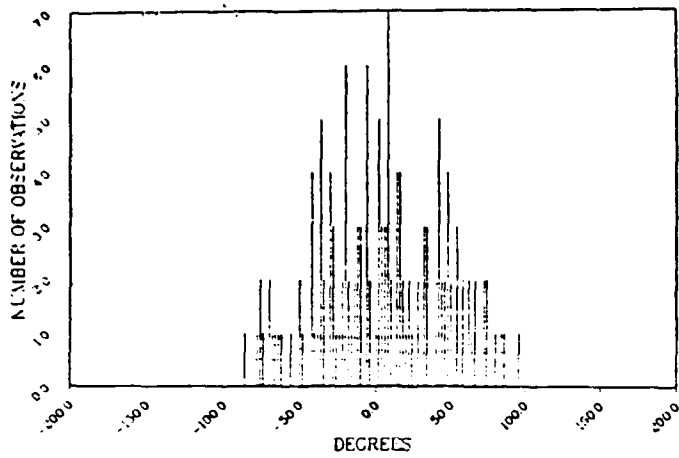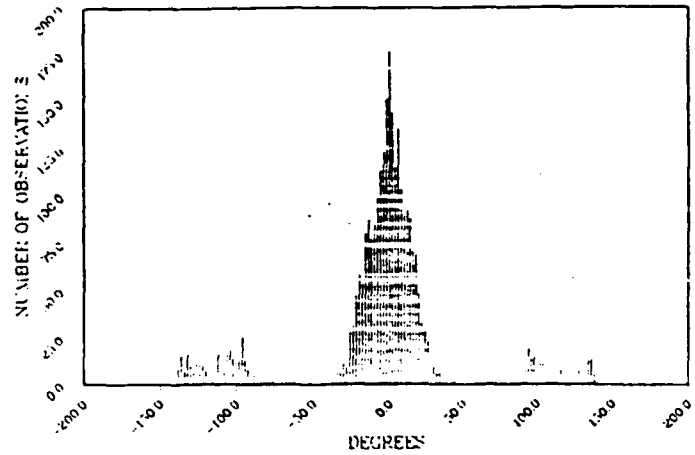
Figure 1

Energy vs. Time

LEGEND

- ■ = Total Energy
- Ⅲ = Kinetic Energy
- ⊞ = Total Potential Energy
- ◫ = Leannard Jones Potential
- ● = Wall Potential
- ○ = Torsional Potential

Time in picosec.

Energy in ergs

$*10^{-12}$

Figure 2
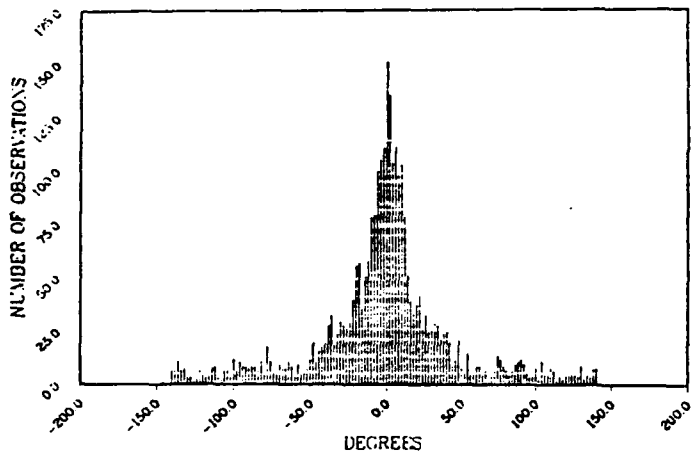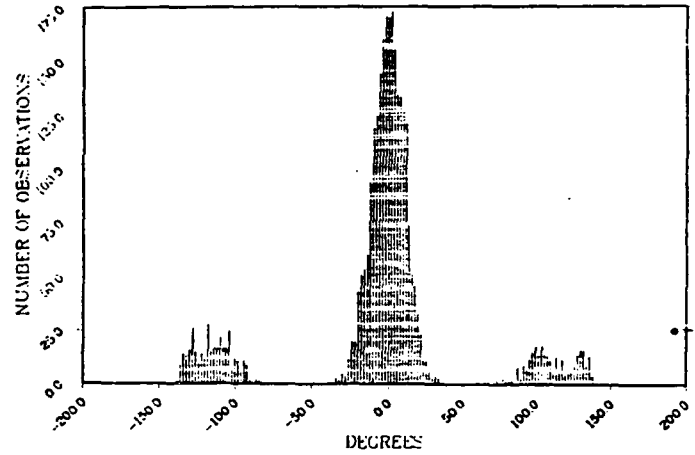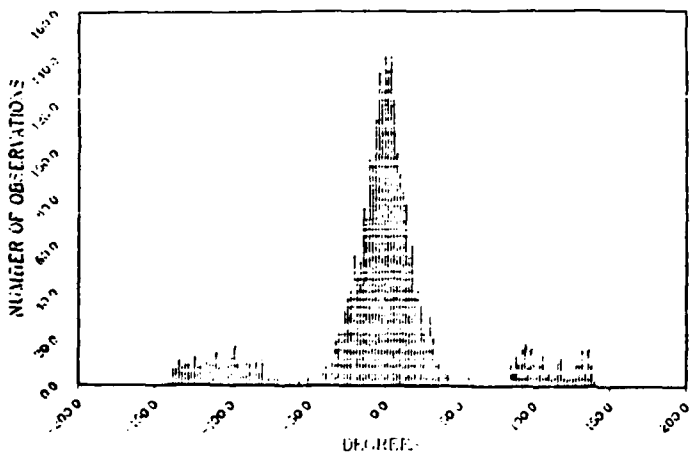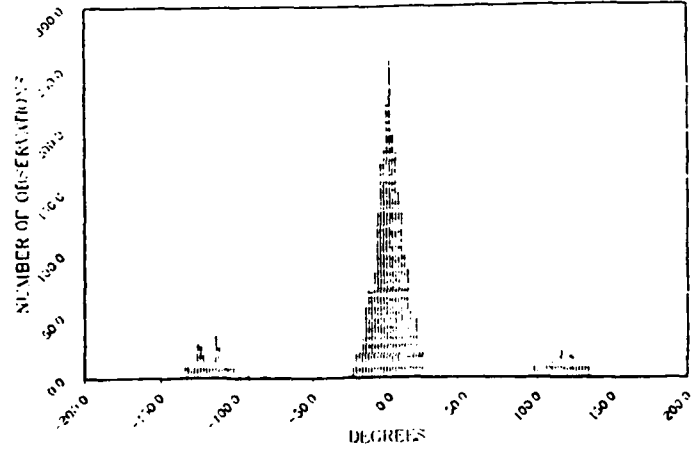
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    Washington, DC 20375

AMZEL, L. Mario
Department of Biophysics
Johns Hopkins School of Medicine
725 North Wolfe Street
Baltimore, MD 21205

ANDERSEN, Niels H.
Department of Chemistry
University of Washington
Seattle, WA 98195

ARNOLD, Frances H.
Dept of Chemical Engineering
California Institute of Technology
Pasadena, CA 91125

AUGUST, J. Thomas
Department of Pharmacology
Johns Hopkins Medical School
725 North Wolfe Street
Baltimore, MD 21205

BEVERIDGE, David L
Department of Chemistry
Wesleyan University
Hall-Altwater Laboratories
Middletown, CT 06457

BRAMSON, H. Neal
Department of Biochemistry
Univ of Rochester Medical Center
601 Elmwood Avenue
Rochester, NY 14642

BRUICE, Thomas C.
Department of Chemistry
University of California-Santa
Barbara
Santa Barbara, CA 93106

CASE, Steven T.
Department of Biochemistry
Univ of Mississippi Medical Center
2500 North State Street
Jackson, MS 39216-4505

CHANG, Eddie L
Bio/Molecular Engineering
Naval Research Laboratory
Code 6190
Washington, D.C. 20375-5000

CHRISTIANSON, David W.
Department of Chemistry
University of Pennsylvania
231 South 34th Street
Philadelphia, PA 19104-6323

CORDINGLEY, John S.
Department of Molecular Biology
University of Wyoming
Box 3944 University Station
Laramie, WY 82071

DeGRADO, William F.
E. I. du Pont de Nemours & Co
Central R & D, Experimental Station
P. O. Box 80328
Wilmington, DE 19880-0328

EVANS, David R.
Department of Biochemistry
Wayne State Univ School of Medicine
540 E. Canfield Street
Detroit, Michigan 48201

FEIGON, Juli F.
Department of Chem & Biochemistry
UCLA
405 Hilgard Avenue
Los Angeles, CA 900024-1569

FICHT, Allison R.
Dept of Med Biochem & Genetics
Texas A&M University
College Station, TX 77843

FRAUENFELDER, Hans
Department of Physics
University of Illinois
Urbana, IL 61801

GABER, Bruce
Naval Research Laboratory
Bio/Molecular Engineering Branch
Code 6190
Washington, DC 20375

GETZOFF, Elizabeth D.
Scripps Clinic & Research Foundation
Department of Molecular Biology
10666 North Torrey Pines Road
La Jolla, CA 92037

GOODMAN, Eugene M.
Biomedical Research Institute
University of Wisconsin
P. O. Box 2000
Kenosha, WI 53141

HO, Pui Shing
Department of Biochemistry and
Biophysics
Oregon State University
Corvallis, OR 97331

HOGAN, Michael E.
Baylor Center for Biotechnology
4000 Research Forest Drive
The Woodlands, TX 77381

HONIG, Barry
Columbia University
Dept of Biochem and Molec Biophys
630 West 168th St.
New York, NY 10032

HOPKINS, Paul B.
Department of Chemistry
University of Washington
Seattle, WA 98195

KAHNE, Daniel
Department of Chemistry
Princeton University
Princeton, NJ 08544

KEMP, Robert G.
Chicago Medical School
Dept of Biological Chemistry
3333 Green Bay Rd.
North Chicago, IL 60064

KHORANA, Gobind H.
Department of Biology
MIT
77 Massachusetts Ave.
Cambridge, MA 02139

KIM, Sangtae
Chemical Engineering
University of Wisconsin
1415 Johnson Drive
Madison, WI 53706

LANSBURY, Peter T.
Department of Chemistry
MIT
Cambridge, MA 02139

LAURSEN, Richard A.
Chemistry Department
Boston University
590 Commonwealth Avenue
Boston, MA 02215

LENZ, Robert W.
Chemical Engineering Department
University of Massachusetts
Amherst, MA 01003

LEWIS, Randolf V.
Molecular Biology Department
University of Wyoming
University Station Box 3944
Laramie, WY 82071

LINDSAY, Stuart M.
Department of Physics
Arizona State University
Temp, AZ 85278

LOEB, George I.
David W. Taylor Research Center
Code 2841
Annapolis, MD 21402-5067

MASILAMANI, Divakar
Biotechnology Department
Allied-Signal Inc.
P. O. Box 1021R
Morristown, NJ 07960

McCONNELL, Harden M.
Stanford University
Department of Chemistry
Stanford, CA 94305

McELROY, Willam D.
Department of Chemistry
University of California - San Diego
La Jolla, CA 92093-0601

MERTES, Kristin Bowman
University of Kansas
Dept of Chemistry
Lawrence, Kansas 66045

NAGUMO, Mark
Bio/Molecular Engineering Branch
Naval Research Laboratory
Code 6190
Washington, DC 20375-5000

OLIVERA, Baldomero M.
Department of Biology
University of Utah
Salt Lake City, UT 84112

PABO, Carl O.
Department of Biophysics
Johns Hopkins University
School of Medicine
Baltimore, MD 21205

·PRENDERGAST, Franklyn G.
Dept of Biochemistry & Molec Biol
Mayo Foundation
200 First St. SW
Rochester, MN 55905

PUGH, Jr., Edward N.
Deaprtment of Psychology
University of Pennsylvania
3815 Walnut Street
Philadelphia, PA 19104-6196

RACKOVSKY, Shalom R.
Department of Biophysics
University of Rochester
School of Medicine and Dentistry
Rochester, NY 14642

RAJAN, K. S.
Illinois Institute of Technology
Research Institute
10 W. 35th St.
Chicago, IL 60616

REINISCH, Lou
Laser Biophysics Center
Uniformed Services University
4301 Jones Bridge Road
Bethesda, MD 20814

RICH, Alexander
MIT Department of Biology
Cambridge, MA 02139

RICHARDS, J. H.
California Institute of Technology
Division of Chemistry and Chemical
Engineering
Pasadena, CA 91125

ROTHSCHILD, Kenneth J.
Department of Physics
Boston University
590 Commonwealth Avenue
Boston, MA 02215

SCHULTZ, Peter G.
Department of Chemistry
University of California-Berkeley
Bekeley, CA 94720

SEEMAN, Nadrian
Department of Chemistry
New York University
New York, NY 10003

SELSTED, Michael E.
UCLA
Dept of Medicine
37-055 CHS
Los Angeles, CA 90024

SIGMAN, David S.
UCLA School of Medicine
Dept of Biological Chemistry
Los Angeles, CA 90024
SIKES, Steven C.
Department of Biological Sciences
University of South Alabama
Mobile, AL 36688

SINSKEY, Anthony J.
Laboratory of Applied Microbiology
MIT Department of Biology
Cambridge, MA 02139

STEWART, James M.
Department of Chemistry
University of Maryland
College Park, MD 20742

STEWART, John M.
Department of Biochemistry
University of Colorado
Health Science Center
Denver, CO 80262

TURNER, Douglas H.
Department of Chemistry
University of Rochester
Rochester, NY 14627

URRY, Dan W.
Laboratory of Molecular Biophysics
University of Alabama
P. O. Box 311
Birmingham, AL 35294

WAITE, J. Herbert
College of Marine Studies
University of Deleware
Lewes, DE 19958

WARD, Keith B.
Naval Research Laboratory
Code 6030
Washington, DC 20375

WARSHEL, Arieh
Department of Chemistry
University of Southern California
University Park
Los Angeles, CA 90089-0482

WATT, Gerald D.
Dept of Chemistry & Biochemistry
University of Colorado
Campus Box 215
Boulder, CO 80309-0215