



Computational Computational Chemistry organic / Inorganic / Physical / Biological

Editors:

Norman L. Allinger
Department of Chemistry
Computational Center for
Molecular Structure and
Design
University of Georgia
Athens, GA 30602-2526

Paul von R. Schleyer Computer Chemistry Center Institut für Organische Chemie Universität Erlangen-Nürnberg Henkestrasse 42, D-91054 Erlangen, Germany

Associate Editor:

Gernot FrenkingFachbereich Chemie
Philipps-Universität Marburg
Hans-Meerwein-Strasse
D-35032 Marburg, Germany

Assistant Editors:

Martin Feigel Institut für Organische Chemie Universität Bochum Universitatsstr. 150 D-44780 Bochum, Germany

Roger S. Grev
Department of Chemistry
University of Kentucky
Lexington, KY 40506

Editorial Production, John Wiley: Merilee Croft Olson

Editorial Advisory Board:

Enrico Clementi Department of Chemistry University L. Pasteur, 3 rue de l'Université 67084 Strasbourg, France

Warren J. Hehre Wavefunction, 18401 Von Karman, Suite 370 Irvine, CA 92715

William L. Jorgensen
Department of Chemistry
Yale University
PO Box 208107
New Haven, CT 06520-8107

Martin Karplus
Department of Chemistry
12 Oxford Street
Harvard University
Cambridge, MA 02138

Peter A. Kollman
Department of Pharmaceutical
Chemistry
School of Pharmacy
University of California
San Francisco, CA 94143

Paul G. Wezey
Department of Chemistry
University of Saskatchewan
Saskatoon, Canada S7N OWO

Keiji Morokuma Department of Chemistry Emory University Atlanta, GA 30322

Eiji Osawa
Department of KnowledgeBased Information
Engineering
Toyohashi University of
Technology
Tempaku-cho, Toyohashi
441, Japan

John A. Pople
Department of Chemistry
Northwestern University
2145 Sheridan Road
Wilmette, IL 60208

Peter Pulay
Department of Chemistry
University of Arkansas
Fayetteville, AR 72701

Leo Radom

Research School of Chemistry The Australian National University Canberra, A.C.T. 0200 Australia

Harold A. Scheraga Baker Laboratory of Chemistry Cornell University Ithaca, NY 14853-1301

Andrew Streitwieser, Jr. Department of Chemistry University of California Berkeley Berkeley, CA 94720

Kenneth B. Wiberg
Department of Chemistry
Yale University
225 Prospect Street
New Haven, CT 06520

Michael C. Zerner Department of Chemistry University of Florida Gainesville, FL 32611

The Journal of Computational Chemistry (ISSN: 0192-8651) is published 16 times a year, monthly and semi-monthly in January, April, July, and November, one volume per year by John Wiley & Sons, Inc.: 605 Third Avenue, New York, NY, 10158.

Copyright © 1998 John Wiley & Sons, Inc. All rights reserved. No part of this publication may be reproduced in any form or by any means, except as permitted under section 107 or 108 of the 1976 United States Copyright Act, without either the prior written permission of the publisher, or authorization through the Copyright Clearance Center, 222 Rosewood Drive, Danvers, MA 01923; tel; 508-750-8400, fax: 508-750-4470. Periodicals postage paid at New York, NY, and at additional mailing offices.

The code and the copyright notice in the journal indicate the copyright holders consent that copies may be made for personal or internal use, or for the personal or internal use of specific clients, on the condition that the copier pay for copying beyond that permitted by Sections 107 and 108 of the United States Copyright Law. The per-copy fee for each item is to be paid through the Copyright Clearance Center, Inc.

This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Such permission requests and other permission inquiries should be addressed to the Permissions Dept.

Subscription price (Volume 19, 1998): \$1,198.00 in US, \$1,358.00 in Canada and Mexico, \$1,475.00 outside North America. \$150.00 US ACS member, \$246.00 outside US ACS member. Personal rate: \$150.00 in US, \$246.00 outside North America. Subscriptions at the personal rate are available only to individuals. All subscriptions outside US will be sent by air. Payment must be made in US dollars drawn on a US bank. Claims for undelivered copies will be accepted only after the following issue has been received. Please enclose a copy of the mailing label. Missing copies will be supplied when

cessing a change of address. For subscription inquiries, please call 212-850-6645; E-mail: SUBINFO@jwiley.com

Postmaster: Send address changes to *Journal of Computational Chemistry*. Caroline Rothaug, Director, Subscription Fulfillment and Distribution, John Wiley & Sons, Inc., 605 Third Avenue, New York, NY 10158. For subscription inquiries, please call customer service at 212-850-6645 or write to the above address.

Advertising: Inquiries concerning advertising should be forwarded to Susan Levey. Advertising Sales, John Wiley & Sons, Inc., 605 Third Avenue, New York, NY 10158, 212-850-8832. Advertising Sales, European Contacts: Bob Kern or Nicky Douglas, John Wiley & Sons, Ltd., Baffins Lane, Chichester, West Sussex PO19 1UD, England, Tel: 44 1243 770 350/367; Fax: 44 1243 Position adsales@wiley.co.uk.

Reprints: Reprint sales and inquiries should be directed to the customer service department, John Wiley & Sons, Inc., 605 Third Ave., New York, NY 10158; tel: 212-850-8776.

Manuscripts should be submitted to one of the editors: Dr. Norman L. Allinger, Journal of Computational Chemistry, Department of Chemistry, The University of Georgia, Athens, GA 30602; Prof. Dr. Paul von R. Schleyer, Journal of Computational Chemistry, Computer Chemistry Center, Institut für Organische Chemie, Universität Erlangen-Nürnberg, Henkestr. 42, D-91054, Erlangen, Germany: or Prof. Gernot Frenking, Journal of Computational Chemistry, Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Strasse, D-35032 Marburg, Germany. Information for contributors appears in the first and last issue of each volume. All other correspondence should be addressed to Journal of Computational Chemistry, Publisher, Interscience Division. Professional, Reference, and Trade Group, John Wiley & Sons Inc., 605 Third Avenue, New York, NY 10158.

The contents of this journal are indexed in the following: Chemical Abstracts, Chemical Titles,



Computational Chemistry

Volume 19/Number 7/Way 1998

CONTENTS	
Development of a Parallel Molecular Dynamics Code on SIMD Computers: Algorithm for Use of Pair List Criterion D. Roccatano, R. Bizzarri, G. Chillemi, N. Sanna, and A. Di Nola	685
Multivariate Analysis of a Data Matrix Containing A-DNA and B-DNA Dinucleoside Monophosphate Steps: Multidimensional Ramachandran Plots for Nucleic Acids M. L. M. Beckers and L. M. C. Buydens	695
Ab Initio Prediction of 15 N-NMR Chemical Shift in α -Boron Nitride Based on an Analysis of Connectivities Marcus Gastreich and Christel M. Marian	716
The Flying Ice Cube: Velocity Rescaling in Molecular Dynamics Leads to Violation of Energy Equipartition Stephen C. Harvey, Robert KZ. Tan, and Thomas E. Cheatham III	726
Systematic Prediction of the Products and Intermediates of Isotopic Labeling in Reaction Pathway Studies Andrew V. Zeigarnik and Raúl E. Valdés-Pérez	741
Electrostatic Model for Infrared Intensities in a Spectroscopically Determined Molecular Mechanics Force Field Kim Palmo and Samuel Krimm	754
Solvation Free Energies Calculated Using the GB/SA Model: Sensitivity of Results on Charge Sets, Protocols, and Force Fields M. Rami Reddy, Mark D. Erion, Atul Agarwal, Vellarkad N. Viswanadhan.	769

(Continued on next page)

Visit Wiley Journals Online
WILEY
InterScience
www.interscience.wiley.com

Volume 19, Number 7 was mailed the week of April 13, 1998

D. Quentin McDonald, and W. Clark Still



Method of Calculating Band Shape for Molecular Electronic Spectra Greg M. Pearl, M. C. Zerner, Anders Broo, and John McKelvey	781
Neighbor-List Reduction: Optimization for Computation of Molecular van der Waals and Solvent-Accessible Surface Areas	797
Jörg Weiser, Armin A. Weiser, Peter S. Shenkin, and W. Clark Still	
Erratum	809



Development of a Parallel Molecular Dynamics Code on SIMD Computers: Algorithm for Use of Pair List Criterion

D. ROCCATANO,¹ R. BIZZARRI,²,³ G. CHILLEMI,² N. SANNA,² A. DI NOLA¹

¹Dipartimento di Chimica, Università "La Sapienza," Ple Aldo Moro 5, 00185 Rome, Italy ²CASPUR Consorzio per le Applicazioni di Supercalcolo per Università e Ricerca, c/o Università "La Sapienza," Rome, Italy

³Dipartimento di Fisica, Università "La Sapienza," Rome, Italy

Received 24 April 1996; accepted 24 October 1997

APR 28 1850

ABSTRACT: In recent years several implementations of molecular dynamics (MD) codes have been reported on multiple instruction multiple data (MIMD) machines. However, very few implementations of MD codes on single instruction multiple data (SIMD) machines have been reported. The difficulty in using pair lists of nonbonded interactions is the major problem with MD codes for SIMD machines, such that, generally, the full connectivity computation has been used. We present an algorithm, the global cut-off algorithm (GCA), which permits the use of pair lists on SIMD machines. GCA is based on a probabilistic approach and requires the cut-off condition to be simultaneously verified on all nodes of the machine. The MD code used was taken from the GROMOS package; only the routines involved in the pair lists and in the computation of nonbonded interactions were rewritten for a parallel architecture. The remaining calculations were performed on the host computer. The algorithm has been tested on Quadrics computers for configurations of 32, 128, and 512 processors and for systems of 4000, 8000, 15,000, and 30,000 particles. Quadrics was developed by Istituto Nazionale di Fisica Nucleare (INFN) and marketed by Alenia Spazio. © 1998 John Wiley & Sons, Inc. J Comput Chem 19: 685-694, 1998

Keywords: molecular dynamics; domain decomposition algorithm; parallel computers; pair list for molecular dynamics code on SIMD machines; array processor elaborator (APE)

Correspondence to: A. Di Nola Contract/grant sponsors: Ente per le Nuove Tecnologie, l'Energia e l'Ambiente; Alenia Spazio

Journal of Computational Chemistry, Vol. 19, No. 7, 685–694 (1998) © 1998 John Wiley & Sons, Inc.

CCC 0192-8651 / 98 / 070685-10



DOCKET

Explore Litigation Insights



Docket Alarm provides insights to develop a more informed litigation strategy and the peace of mind of knowing you're on top of things.

Real-Time Litigation Alerts



Keep your litigation team up-to-date with **real-time** alerts and advanced team management tools built for the enterprise, all while greatly reducing PACER spend.

Our comprehensive service means we can handle Federal, State, and Administrative courts across the country.

Advanced Docket Research



With over 230 million records, Docket Alarm's cloud-native docket research platform finds what other services can't. Coverage includes Federal, State, plus PTAB, TTAB, ITC and NLRB decisions, all in one place.

Identify arguments that have been successful in the past with full text, pinpoint searching. Link to case law cited within any court document via Fastcase.

Analytics At Your Fingertips



Learn what happened the last time a particular judge, opposing counsel or company faced cases similar to yours.

Advanced out-of-the-box PTAB and TTAB analytics are always at your fingertips.

API

Docket Alarm offers a powerful API (application programming interface) to developers that want to integrate case filings into their apps.

LAW FIRMS

Build custom dashboards for your attorneys and clients with live data direct from the court.

Automate many repetitive legal tasks like conflict checks, document management, and marketing.

FINANCIAL INSTITUTIONS

Litigation and bankruptcy checks for companies and debtors.

E-DISCOVERY AND LEGAL VENDORS

Sync your system to PACER to automate legal marketing.

