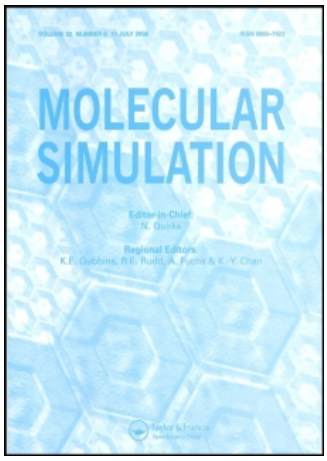
This article was downloaded by:[New York University]
[New York University]
On: 16 July 2007
Access Details: [subscription number 769426389]
Publisher: Taylor & Francis
Informa Ltd Registered in England and Wales Registered Number: 1072954
Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

A Near-neighbour Algorithm for Metropolis Monte Carlo Simulations

Mihaly Mezei [a]
[a] Department of Chemistry and Center for Study in Gene, Structure and Function. New York, NY. USA

Online Publication Date: 01 March 1988
To cite this Article: Mezei, Mihaly , (1988) 'A Near-neighbour Algorithm for Metropolis Monte Carlo Simulations', Molecular Simulation, 1:3, 169 - 171
To link to this article: DOI: 10.1080/08927028808080940
URL: http://dx.doi.org/10.1080/08927028808080940

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.informaworld.com/terms-and-conditions-of-access.pdf

This article maybe used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

© Taylor and Francis 2007

Molecular Simulation, 1988, Vol. 1, pp. 169–171
Photocopying permitted by license only
Reprints available directly from the publisher
© 1988 Gordon and Breach Science Publishers, S.A.
Printed in Great Britain

A NEAR-NEIGHBOUR ALGORITHM FOR METROPOLIS MONTE CARLO SIMULATIONS

MIHALY MEZEI

Department of Chemistry and Center for Study in Gene Structure and Function, Hunter College of the CUNY, New York, NY 10021, USA

(*Received December 1986; in final form April 1987*)

A bit map based implementation of a near-neighbour algorithm to speed up Metropolis Monte Carlo simulations is described. Tests of the algorithm on dilute aqueous solutions showed 8%–22% overall reduction of computer time, depending on the system size.

KEY WORDS: Monte Carlo computer simulation, near-neighbour algorithm, bit map.

INTRODUCTION AND BACKGROUND

Monte Carlo computer simulations are routinely performed on molecular assemblies of 0(100) molecules. These calculations are rather long: they consume 50–100 hours of mainframe time. A customary procedure to keep computer time down is the application of a spherical cutoff on the interaction potential – molecules that are further apart than a certain threshold distance (cutoff) are considered to have zero interaction energy. This reduces the number of interactions to be computed. However, as the size of the simulation cell is increased in comparison to the cutoff value, an increasing proportion of the time will be spent on calculating distances (under the customary periodic boundary conditions, this is somewhat time consuming).

Near-neighbour algorithms are designed to eliminate most of the unnecessary distance calculations by keeping track of the molecules that are in each other's neighbourhood. The difficult part in designing such an algorithm is the efficient maintenance of this information as the molecules move. Generally, published algorithms deal with dynamical systems where all particles move simultaneously and are designed to reduce the number of interaction calculations from $O(N^2)$ to $O(N)$ [1]. The advent of supercomputers introduced an additional aspect, the problem of vectorization: algorithms that are optimal on a scalar machine may fare worse on a vector machine [2]. The comparison of algorithms is further complicated because their performance depends both on the physical problem at hand and on the computer used [3].

The Metropolis Monte Carlo technique [4] presents the additional difficulty that at each step only one molecule is moved; thus, the relative cost of updating the neighbourhood informations generally becomes worse. This communication describes a (vectorizable) way to perform efficiently "local" updates using a bit map to keep track of neighbours. Results of tests on aqueous solutions are also presented.

DESCRIPTION OF THE ALGORITHM

Let us denote by $r_{i,j}$ the distance between molecules i and j, by R_c the interaction cutoff, by R_{nn} the threshold distance for neighbour definition ($R_{nn} > R_c$), and by d_{max} the maximum distance a molecule can move in one step.

1. Establish a 0–1 matrix $B_{i,j}$ (bit map) such that

$$B_{i,j} = \begin{cases} 0 \text{ if } r_{i,j} > r_{nn} \\ 1 \text{ if } r_{i,j} \leqslant r_{nn} \end{cases} \quad (1)$$

2. Set the components of the molecular displacement vector $\mathbf{D}_i$ for each molecule to zero.
3. When a molecule is displaced (attempted move), update the displacement vector of that molecule and check if its new magnitude is larger than $(R_{nn} - R_c)/2$. If it is not, continue with step 5.
4. For molecule i, calculate all distances $r_{i,j}$, update the corresponding values in the bit map $B_{i,j}$ (row i and column i) and save the current position into $\mathbf{C}_i$.
5. For the calculation of the energies, compute distance only for (i, j) such that $B_{i,j} = 1$.
6. Repeat from step 3 for the next displacement.

RESULTS AND DISCUSSION

The algorithm has been tested in our Monte Carlo program using the Metropolis method [4] with force-biased displacement [5] and preferential sampling around the solute [6] on two different systems. The first system contained one small solute (glycine zwitterion, as described by the potential library of Clementi and co-workers [7, 8]) and 215 water molecules (MCY-CI potential [9] with $r_c = 7.75$ Å) under face-centered cubic periodic boundary conditions, while the second system consisted of one DNA tetramer duplex and 792 waters with $r_c = 6$ Å in a hexagonal prism (again, using periodic boundary conditions). For both cases, $r_{nn} = r_c + 2$ Å was employed. This resulted in 50% and 90% of the waters being outside the neighbourhood sphere for the 215 and 792 water systems, respectively. The maximum water stepsize was 0.275 Å for both systems. An 8% reduction in the total run time was obtained for the first system and a 22% reduction for the second. The gain on the glycine system remained the same for $r_c + 1.5$ Å $\leqslant r_{nn} \leqslant r_c + 2$ Å. The frequency of bit map updates turned out to be at every 100 configurations on the average. The possible relaxation of the update condition in step 3 has also been tested and it was found that even minor relaxation would lead to incorrect energy values within 10^6 configurations.

The saving in computer time is already significant in the present implementation, since a simulation on such aqueous systems requires 10–100 hours of present-day mainframe computer time. However, the above results can probably be significantly improved if the currently implemented bit manipulations using integer, logical and modulo operations are replaced by an assembler routine. Furthermore, since the data to be accessed is linearly spaced in the array $B_{i,j}$, the code will easily vectorize. It may suit particularly well the Cyber-205, since this machine provides a vectorized access to an array when the items to be used are controlled by a bit map.

On the negative side, at each step one still has to look at all N neighbours, even if briefly in most cases, and the memory requirement of the bit map is N^2/(bits per computer word) computer word. Thus, for very large systems or for very simple potentials the algorithm is not likely to be efficient. This disadvantageous limiting behaviour, however, did not degrade the performance for a system 0(1000) molecules.

A priori comparisons with other methods cannot be obtained since the efficiency of the present method depends strongly on the update frequency, which is a function of the physical system at hand. Dense fluids, where the movement of the particles is largely oscillatory, appear to be able to take advantage of the present algorithm.

Acknowledgements

This research was supported by NIH grant GM 24914, NSF grant CHE-8293501 and RCMI grant #SRC5G12RR03037 from NIH to Hunter College, CUNY. Several useful discussions with Professor K. Bencsath are gratefully acknowledged. The referee is thanked for suggesting the use of molecular displacement vectors in Step 3.

References

[1] R.W. Hockney and J.W. Eastwood, *Computer Simulation Using Particles*, McGraw-Hill, New York, 1981.

[2] J. Boris, "A vectorized 'near neighbours' algorithm of order N using a monotonic logical grid," *J. Comput. Phys.*, **66**, 1 (1986).

[3] W.F. van Gunsteren, H.J.C. Berendsen, F. Colonna, D. Perahia, J.P. Hollenberg and D. Lellouch, "On searching neighbours in computer simulation of macromolecular systems," *J. Comput. Chem.*, **5**, 272 (1974).

[4] N.A. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, "Equation of state calculation by fast computing machines," *J. Chem. Phys.*, **21**, 1087 (1953).

[5] M. Rao, C.S. Pangali and B.J. Berne, "On the force bias Monte Carlo simulation of water: Methodology, optimization and comparison with molecular dynamics," *Mol. Phys.*, **37**, 1779 (1979).

[6] J.C. Owicki and H.A. Scheraga, "Preferential sampling near solutes in Monte Carlo calculations on dilute solutions," *Chem. Phys. Lett.*, **47**, 600 (1979); J.C. Owicki, "Optimization of sampling algorithms in Monte Carlo calculations of fluids," in *Computer Modeling of Matter*, P.G. Lykos, ed., American Chemical Society, Washington, DC, 1978.

[7] E. Clementi, F. Cavallone and R. Scordamaglia, "Analytical potentials for 'ab initio' computations for the interactions between biomolecules. 1. Water and amino acids," *J. Am. Chem. Soc.*, **99**, 5531 (1977).

[8] S. Romano and E. Clementi, "Monte Carlo simulation of water solvent with biomolecules. Glycine and the corresponding zwitterion," *Int. J. Quant. Chem.*, **XIV**, 839 (1978).

[9] O. Matsuoka, E. Clementi and M. Yoshemine, "CI study of the water dimer potential surface," *J. Chem. Phys.*, **64**, 1351 (1976).