MELQUIADES: A Monte Carlo program for simulation of multicomponent systems using arbitrary potential models

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INTRODUCTION

A general purpose Metropolis Monte Carlo program, for the simulation of multicomponent system is presented.

METHODS

MELQUIADES is a serial and stand-alone FORTRAN 90/95 program for simulation of multicomponent systems using Metropolis Monte Carlo Algortihm[1]. It can be compiled using the GNU Fortran Compiler (gfortran) 4.8 in different GNU/Linux distributions and hardware. In the current version some capabilities implemented are: i) besides Coulombic potential, Lennard-Jones, Buckingham or Yukawa potentials[1,3] to can be used to calculate intermolecular interaction energy; ii) the configuration space is sampled either in canonical or isothermal-isobaric ensembles; iii) allows the multicomponent system energy calculation and building of diverse neighbor list depending on the molecular size; iv) the trajectories can be saved in xyz and/or xtc format file; v) interfaces with the plotting tools gnuplot or xmgrace and molecular visualization program vmd, molden are available. The source code of MELQUIADES was written in modular format as to facilitate the inclusion or adaption of other potential models or analysis tools.

RESULTS AND DISCUSSION

In this work, the capacity to simulate multicomponent systems is shown through the calculation of the intermolecular interaction energy between water molecules using the TIP3P transferable model. The calculations were carried out on the canonical ensemble at 298 K, using periodic box boundary conditions with a central box filled with 2048 TIP3P molecules.

Fixing the total number of molecules, the test consisted on the calculation of the average interaction energy per molecule assuming that the simulation box is divided into 1, 2, 4, and 8 components with the same number of molecules. Therefore, in such arrangement, the average interaction energy per molecule must by the same within the statistical error. In all calculations the average energy per molecule obtained was -9.81 kcal/mol with standard deviation 0.00106, in good accord with the values reported in the literature. The figure 1 show the run-time value in seconds for calculations performed with different number of components and size of the markov chain. In figure 1, blue and red lines represents, respectively, markov chain with $1x10^5$ and $2X10^5$ configurations. One observes that, for a given markov chain size, the computer time is independent of the number of components. Some fluctuations, in the order of microseconds, associated to machine architecture were observed.

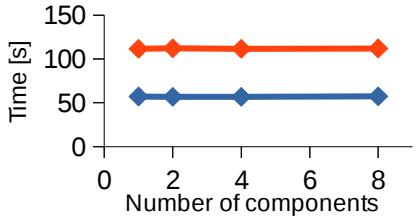

Figure 1. Run-time in markov chain

CONCLUSIONS

The MELQUIADES program can be used for the simulation of complex mixtures. The present test indicate negligible influence of the number of components on the average values and the computer run time.

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