ERGODICITY OF PARALLEL CALCULATED TRAJECTORIES MOLECULAR DYNAMICS

V.N. Petrov* , K.V. Shaitan
M.V. Lomonosov Moscow state university, Biological faculty

At calculations by a molecular dynamics method it is important that the obtained trajectories gave statistically authentic outcomes. The trajectories will have sufficiently property of ergodicity, if during a simulation an imaging point will visit the enough number of times all units of substantially accessible of configuration space. The most difficultly accessible areas separated by potential hills, which characteristic height for conformational labile systems makes a little (less than 10) kkal/mol. So, at height of a barrier 10 kkal/mol and T=300K the characteristic time of overcoming of a barrier makes about 10 μs. Molecular dynamics trajectories lengths do not exceed, as a rule, 10ns. However areas of conformation space separated by such barriers can be significant from the point of view of substantial processes happening in biopolymers, as characteristic times of many enzymatic responses about milliseconds and more. At temperatures about 2000 - 2500K the characteristic time of overcoming of such barrier for oligopeptides is reduced up to 10ps. The estimates show, that in this case for rather small peptide systems on trajectories of length 10ns it is possible to receive statistically quite reasonable outcome. Let's mark, that such increase of temperature at the selected system of potentials does not lead to corrupting a molecule. The increase of temperature has an effect only for increasing of amplitudes of thermal fluctuations of lengths of valence bonds, values of valence angels and acceleration of a hindered rotation around of chemical bonds.

The further acceleration of calculation of a trajectory is possible to realize molecular dynamics trajectories by splitting it on some small trajectories and subsequent start of parallel calculation. Thus such trajectories should start from different areas of conformation space of the calculated system. The start points become during calculation of a molecular dynamics trajectory at temperatures about 5500-6000K at regular intervals. For research of ergodicity of systems by splitting one lengthy trajectory on a little bit small calculations, a number of limiting hydrocarbons ethane – decane are used. For each molecule the packages from 100 trajectories with length 0.1ns were calculated at temperature 1500K (starting points were obtained as a result of calculation of a trajectory at temperature 4500K through intervals in 10ps) and at temperature 500K (the starting points were obtained as a result of calculation of a trajectory at temperature 3000K through intervals in 10ps), and as individual trajectories by lengthy 10ns at 1500K and 500K. The comparison is carried out between the packages and individual trajectories obtained at corresponding temperatures. The comparison is carried out by one-dimensional probability distributions, auto- and crosscorrelation functions of dihedral angels, where the one-dimensional probability distributions, auto- and crosscorrelation functions of dihedral angels in packages of trajectories were calculated by the following ways: 1. simple averaging of the data. 2. averaging of the data with a statistical weight of initial potential energy of each trajectory 3. averaging of the data with a statistical weight of average potential energy of each trajectory.

The calculation has shown that with increase of number of dihedral angels in a molecule the difference between the package of trajectories and individual trajectory are enlarged. At temperature of calculation 500K it happens faster, than at 1500K. Simple averaging of the data and averaging of the data with a statistical weight of average potential energy of each trajectory give the best outcomes.

The work is partially supported by RFFI (01-04-49302), Ministry of Industry, Science, and Technology RF (40.165.11.0102) and the Ministry of Education RF (I-0431).