A HIGH PERFORMANCE SYSTEM FOR MOLECULAR DYNAMICS SIMULATION OF BIOMOLECULES USING A SPECIAL-PURPOSE COMPUTER

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Molecular dynamics (MD) simulation is recognized as a promis approach to analyze the physico-chemical nature of biomolecu Computational demand for MD of biomolecules is enormous, however. Hence, a rapid MD system was constructed in which nonbonded interactions, the most time-consuming of MD, was computed by a special purpose computer named MD-GRAPE (GRAvity PipE for MD).

MD-GRAPE is a special purpose computer for N-body simulations of classical particles. MD-GRAPE is loaded with eigh newly developed LSIs named MD-chip. An MD chip treats 6 particles simultaneously; hence, 48 particles are subject to pa computation in MD-GRAPE. The peak speed of MD-GRAPE is 6 Gflops at a clock cycle of 25 MHz. MD-GRAPE handles any kind central force and potential such as Coulomb interactions. MD-GRAPE is connected to a host workstation through a bus adapte an N-body simulation, MD-GRAPE performs companions proportional to N^2, while the host performs those proportiona

First of all, the performance and precision of MD-GRAPE w tested by MD of several non-dimensional particle systems. Th effective speed of MD-GRAPE was 6 Gflops when N >10,000, abo

13 times faster than Cray C90 and 160 times than DEC 3000/ the host workstation. The precision of MD-GRAPE was good enc judging from the fluctuation in total energy.

Next, a software package named PEACH (Program for Energetic Analysis of bioCHemical molecules) was developed fo molecular dynamics of biomolecules in combination with MD-GRAPE. PEACH consists of several modules and the data are transmitted among the modules via files The module MKDBAS makes a database of residues, MKMOL constructs the topology the molecule, MKCOR makes the coordinates, adds solvents, anc on, and finally MKPARA assigns the force field parameters. RUNMD performs MD by using files made by MKCOR and MKPARA In RUNMD, Coulomb and van der Waals interactions are calcula by MD-GRAPE. Integration scheme is Velocity-Verlet. PEACH is written in Fortran90.

Finally, MD simulation was performed for several protein-solvent systems, A-C, with different sizes (N~ 3,200 for system ~10,000 for system B, and ~27,000 for system C) to test the performance and precision of the PEACH-GRAPE system. Computation time per each time step was 0.8 (system A), 1.6 (system B), and 5.5 s/step (system C), and acceleration of the by MD-GRAPE was 24, 91, and 213 fold, respectively. Thus, the performance of the PEACH-GRAPE system without the cut-off scheme was as fast as the current supercomputers using the approximation. The precision of the PEACH-GRAPE system was good comparing the fluctuation in total energy during MD wit of the host. Thus, the PEACH-GRAPE system is expected to be useful in accurate and reliable simulation of large biomolecule