Parallel Molecular Dynamics Simulation for Very Large Molecules

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Abstract

Computer simulation on advanced high performance computers is important in science and technology. Since parallel computers containing many processing elements (PEs) have huge computational ability, parallel computers come to be used for various types of computer simulation. However, parallel computers have a problem about difficulty of parallelization method. This thesis addresses parallelization method of Molecular Dynamics (MD) simulation. MD is used in physics, chemistry, and material science fields as an important simulation method. MD deals with various molecules, especially very large molecules are simulated on parallel computers only. Parallel 3-dimensional MD simulations have following three problems for a large number of molecules.

Firstly, analytic formula of parallel execution time is required for general case. We formulate theoretical parallel execution times of domain decomposition method (DDM) on message-passing parallel computers. The theoretical formulae of parallel execution time decide the optimal domain shape of DDM among three available domain shapes, and the theoretical execution times are in agreement with the experimental results on parallel computers.

Next, computational load balancing in parallel computers is important to achieve efficient parallel simulations. We propose a dynamic load balancing method (DLB) based on task scheduling. DLB uses a cell as the unit of task, and a principle of "permanent cells" is introduced into DLB to keep PEs' neighboring relationship symmetric. DLB achieves computational load balancing in 3-dimensional simulation with keeping PEs' neighboring relationship regular.

The third problem is the parallelization of intra-molecular interaction. Chain molecules contain many linearly connected "monomer", and the molecules have intra-molecular interaction. Intra-molecular interaction in DDM requires search for connected monomer, and the search increases the total execution time. For MD simulation of chain molecules, DDM with chain pieces distribution (CDDDM) is proposed in order to reduce monomer search. CDDDM reduces whole of the execution time with decreasing monomer search.

Key Words: **massively parallel computer, Molecular Dynamics, interprocessor communication time, dynamic load balancing, chain molecule**