Fast Molecular Dynamics Simulation on a Parsytec PowerXplorer System

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The aim of molecular biology is to understand the relationship between structure and function of biological molecules, i.e., proteins, lipids or nucleic acids. In the recent decade it became clear that the motion of individual atoms plays a crucial role in determining many aspects of molecular properties. Since this motion is hard to observe in experiments directly, one has to use a sufficiently realistic model to obtain detailed insight into the dynamics at an atomic level.

One successfull model is to represent atoms as pointmasses with partial electric charges and describe chemical interactions by a semi-empiric force field. Typically, the force field is composed of short range forces (bonding forces, angle forces, etc.) acting between chemically bonded atoms and long range forces, i.e., Coulomb interaction, which couples all partially charged atoms. The computational effort of the short range forces increases linear with the number N of atoms and is for sufficiently large systems ($N > 100$) negligible compared to the computational effort caused by Coulomb interaction, which increases with N^2. The classical Newtonian equations of motion can be solved numerically to obtain the time-development of the model system. This approach is called the molecular dynamics (MD) simulation [?, ?, ?]. Due to the numerical effort of this approach the simulated time span of MD simulations is restricted to 1 ns.

Most of the biologically interesting timescales for MD simulations lay beyond a few nanoseconds and range up to several seconds. To avoid numerical errors, the integration time step must not be much larger than approximately

1 fs, a time which is dictated by the fastest motions in the molecule. For the calculation of only 1 ns of simulated time, one million integration steps have to be performed.

Realistic MD simulations of proteins should also include a part of the natural surrounding of the protein. Usually biological macromolecules are embedded in an enviroment of water or lipids. In our research group we study the membrane protein *bacteriorhodopsin*, which converts light energy into biologically usuable energy. Figure 1 [?] shows a model of *bacteriorhodopsin* (green), which has been embedded into a membrane-water system, totalling about 35,000 atoms. The membrane consists of 200 lipids. Each lipid is composed of a headgroup (yellow) and two carbon chains (grey). On the two sides of the membrane several layers of water molecules (orange and red) have been placed.

-bb-error =

null

Figure 1: Model of *bacteriorhodopsin*, which is embedded in his natural surrounding, i.e. a lipid membrane and water.

For one pair interaction roughly 50 floating point operations have to be evaluated. To simulate realistic systems composed of several 10,000 atoms over interesting time spans, which are longer than 1 ns, more than 10^{16} floating point operations have to be performed. To obtain results in tractable times we employ parallel computers, in particular a 16 node PowerXplorer system from Parsytec, and efficient algorithms for an approximate evaluation of long range forces.

Various studies [?, ?] have shown that in MD simulations an approximate calculation of Coulomb interactions can be used to speed up the computations. Therefore we developed the program EGO_VIII[1] [?, ?, ?] which combines a *Fast Multipole Method* (FMM) [?, ?, ?] and a *Multiple Timestep Method* [?, ?] for rapid, yet stringent evaluation of Coulomb interactions. The FMM is based on a multipole expansion of the Coulomb potential to a given order for a hierarchical subdevision of space. Rather than to use a cubic subdevision of space as most implementations of the FMM do, we did choose a *Structure Adapted* [?] decomposition. This method takes advantage of knowledge about structural and dynamical features of the biomolecules and helps to reduce the computational effort. The *Multiple Timestep Method* is based on the fact that the influence of far seperated atoms varies slowly with time and, therefore, the contribution of these interactions can be evaluated

[1]The program EGO_VIII is written in the programming language C.

less frequently. The combination of these algorithms we call *FAst MUltiple timestep Structure Adapted Multipole Method* (FAMUSAMM) [?].

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Figure 2: Scaling performance of EGO_VIII for a PowerXplorer system with 16 nodes.

For systems with more then 30,000 atoms we achieved a speedup of factor 60 compared to an exact evaluation of the Coulombic forces. In spite of this algorithmic speedup the computational effort still is immense and massive computer power is needed. For that reason the program EGO_VIII has been implemented on parallel computers, in the course of which two versions of EGO_VIII emerged: As we are using a PowerXplorer parallel computer in our institute, one version of the program utilizes PARIX [?] for an optimized message passing between the nodes. In figure 2 the achieved speedup for a various number of atoms is shown. The second version of EGO_VIII uses PVM [?] , which guarantees compatibility to many other parallel computers.

On a PowerXplorer with 16 nodes one integration step for the above described protein–membrane system takes about 3 seconds. So we are now able to calculate 1 ns simulation time of this system in about one month computation time. Two years ago a MD simulation of a membrane system [?] consisting of 25,000 atoms took about two years for a simulation time of 0.2 ns.

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