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The GROMACS and NAMD Software Packages Comparison

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Abstract. The comparable feature analysis of NAMD and GROMACS molecular dynamics packages has been done. The benchmarks of 72 and 128 Dipalmitoylphosphatidylcholine (DPPC)/water have been constructed using a cluster (3GHz-Xeon processors and Myrinet network) and the comparison has been performed using GROMOS87 and CHARMM27 force fields modified for lipids with GROMACS and NAMD software packages, respectively. The GROMACS has been displayed as faster than NAMD, likely due to united-atom character of GROMACS and good implementation features. The GROMACS reaches saturation and goes to the worst results, the reason of which is that the program spends more time on communications between processors.

Key words: NAMD; GROMACS; molecular dynamics; phospholipid bilayers.

1 Introduction

The usage of Molecular Dynamics (MD) simulation in phospholipid bilayers, the main structural elements of cell membranes, makes it possible to study the physical and chemical processes inside of a bilayer and follow directly the conformational changes, to measure all the parameters and compare with the experimental findings. For this reason, any software package, which in a manner regards to the biophysical problems, namely to phospholipid membranes, are of a great interest. There are a lot of famous MD software packages, such as GROMACS [1,2], NAMD [3], CHARMM [4], AMBER [5], TINKER [6], and a lot of

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different force fields modified for various systems are developed. It is reasonable to divide existing software packages into 2 major categories: (i) Computational (ii) 2D and 3D Construction. Computational software packages include molecular mechanics using various force fields, as well as *semi-empirical* and *ab initio* quantum mechanical calculations, such as GAMESS [7], MOPAC [8], GAUSSIAN [9], etc. In addition to calculation tools, in many cases the packages include also constructions, visualization and some drawing tools, being multi-purpose packages. Most of them are designed to be run generally under Unix/Linux platform, although, the Windows platform based computational softwares are also available, like HyperChem [Hypercube, *Inc*], etc. As for the visualization software, it should be noted that there are widely-used, free packages, like Rasmol and VMD [10]. These are programs for displaying, animating and analyzing large bio-systems by means of 3D graphics and scripting. The VMD code is an excellent tool, especially for lipid bilayer assemblies, which provides a wide collection of various methods for rendering, and even MD trajectory analyzing tools are already developed.

Thus, a great deal of progress has been made in the past decade, from the software point view. The purpose of the present research is a comparison of features of such known MD software packages, as NAMD and GROMACS, which are aimed at the high performance simulation with parallel support.

2 Results and discussion

Some comparison of the software properties is presented in Table 1. The main difference is surely the implementation type and force fields. There are also great differences in case of parallel running. As GROMACS developers claim "fastest MD" in some manner according to our calculations, GROMACS is certainly faster than NAMD; however, the latter scales well in parallel performances [11]. GROMACS offers a lot of analysis module, whereas NAMD has almost no standard tools for analysis, which indeed creates some additional troubles for users having no programming facilities.

The GROMACS uses the GROMOS force field and their modifications, and NAMD has an ability to work with CHARMM, X-PLOR, AMBER and even GROMACS force fields. As far as the GROMACS and AMBER force fields support is concerned, it has some major difficulties and practically it is impossible to launch NAMD with GROMACS force field, e.g. to deal with lipids. The main problem is the restrictions, i.e. NAMD does not support many specific tools and configuration options, such as GROMACS pairs section, exclusions, all types of bond potentials, which exist in GROMACS, etc., although NAMD developers have pointed out that only GROMACS topology (.top) and coordinate (.gro) files are needed.

The GROMACS performs the *energy minimization* by means of two various methods: *steepest descent and conjugate gradient* (Polak-Ribiere) methods. The NAMD offers only one standard method for energy minimization (efficient conjugate gradient, which is claimed a faster minimizer algorithm based on the conjugate gradient method).