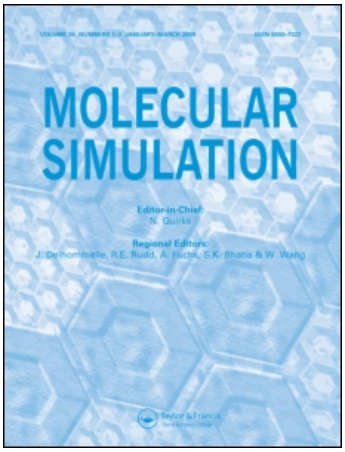

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Note: NAMD-LP: Filtering and Translating NAMD-generated Files

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Note

NAMD–LP: Filtering and Translating NAMD-generated Files

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INTRODUCTION

Currently, science is in a technological boom with many new and improved scientific tools entering the marketplace. The instruments that have existed for decades have seen improvements in sensitivity and accuracy, as well as complexity. Even the newly-developed instruments are complex. As time progresses, these tools will become more complex with added features. This is not only true for instruments, but also computer-assisted science. The use of computers has become ubiquitous and even spawned a new aspect of science, *in silico* analysis and modeling. Computers are quickly growing in computational capabilities allowing more tools to be created and used by researchers, especially research-oriented software. One such area that is benefiting from this technological boom is that of computational macromolecular modeling. This field did not exist a few decades ago, but has since developed because of the capabilities computers now have. Currently, the software that is available is relatively sparse.

There are three types of research-oriented software users—those who are capable of programming, those who are willing to try some programming, and those who want the software to work with no effort needed. The number of scientists who would classify in each category exponentially increases from the first to the last category listed. Probably, greater than ninety-eight percent of researchers would be classified in the last category. Unfortunately, today's free software for molecular modeling requires users to be classified in one of the first two categories. For the last category of users, some software is available at a high cost.

In the area of molecular modeling, one available tool is NAMD [1]. NAMD is a program for scientists to accurately optimize and refine protein structural models and is available on many operating systems, including Linux, MacOS, and Windows. NAMD generates an unwieldly log file that a researcher can manually sort to determine accuracy of an execution. For Linux, NAMD has a component known as NAMD Plot. However, many researchers have difficulty with getting NAMD Plot to operate. If the user's configuration is not exactly the same as the programmer's configuration, then problems arise. Therefore, NAMD Log Parser was created in Java to overcome these dependencies and allow for cross-platform compatibility. NAMD Log Parser is freely available and created for all categories of researchers.

OVERVIEW

Since NAMD is available for many different operating systems, NAMD Log Parser (NAMD–LP) also needed to operate on the same operating systems. Therefore, Java was selected as the programming language. Many programmers do not use Java since it requires an interpreter, which causes a decrease in processing speed. NAMD–LP is not processor intensive, thus not suffering from an operating deficiency caused by the Java interpreter. In addition, Java allows a single file for distribution of the program for all operating systems.

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NAMD–LP is organized into three main functions—data import, data graphing, and data export. Data import will read a NAMD log file and retrieve only the pertinent information. To describe the importance of such filtering, an example file will be described. This example file was generated by NAMD version 2.5b2 and is an ASCII text file approximately 3.12 MB in size. It is a total of 27,280 lines. The pertinent data for the researcher was generated for the first 8000 cycles, then once for every 1000 cycles until reaching 38,000 cycles. For each cycle, only one line contains pertinent information. Thus, less than thirty percent of the file contains information pertinent for a researcher and would be difficult and time consuming to sort through manually.

Once NAMD–LP has filtered and extracted the data, the other two functions are usable. The graphing capabilities are minimal, but allow the researcher to view quickly the progress of a NAMD simulation while NAMD is still working. Some simulations can take days or even weeks to run depending on the computer architecture; therefore, it is very important to monitor the progress of a simulation graphically during this long period of time. Only one variable can be selected for the *x*-axis and one for the *y*-axis. NAMD–LP will display the graph so that it is utilizing the entire program window. In addition to showing the graph, the data can be exported in two fashions, as raw data and as a graph. When the data are exported as the raw data, NAMD–LP will create a tab-delimited text file that can be opened in many programs, such as SigmaPlot, OpenOffice Calc, and Microsoft Excel. Also, the graph of the data can be saved as an encapsulated postscript (EPS), JPEG, or portable network graphic (PNG) file. The EPS file is a vector-based graphics file allowing the image to be enlarged with no loss of quality. However, an EPS file is not as widely accepted as a JPEG or PNG file.

The three main functions of this program can be seen in the program design. The user instructs the program of the location of the NAMD log file. Once imported, the raw data are displayed in the "Data" tab. The "Graph" tab displays the graph of the users chosen *x*- and *y*-axis. The exporting of the data and the graph is under the "Export" tab.

For additional information about NAMD Log Parser, please read the instruction manual included with the program and visit the website (http://namd-lp.sourceforge.net/).

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