A New Software For Visualization of Large Proteins

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1 Abstract

Studies of interaction between protein molecules sometimes require visualizing huge numbers of atoms in a molecular graphics pictures. Namba et al.[1] has reported that simplification and enhancement makes molecular pictures informative in their structural study of protein and nucleic acid in the tabaco mosaic virus. Their pictures have boundary outlines to distinguish different monomers which are symmetrically packed to form the virus, but it is not accomplished by currently available molecular graphics softwares. As novel research in structure biology increased, we will need more functions for graphics software to meet our biological interest. However most software are hard to modify and not expected to be improved on a specific request.

A new software development project of an extensible protein visualization program for structure analysis and prediction study has started for this demand. Our goal is to provide a software platform which runs on common hardware and allow users to add new functions with average programming skill. Our first version is a structure viewer program of proteins in PDB database.

In this project, an application supporting library was designed together with a target program to lead clear prospect of the complicated programming. Among number of technical issues for building a graphics software, 3d-graphics library and memory management functions are redesigned for fast drawing of large number of atoms. An original plug-in module function and a graphical user interface tool kit is also designed. This plug-in module was implemented by dynamic linking system calls in Unix system. The program can be configured with necessary modules from numbers of viewing and analysis functions for the software which we will develop eventually. Also a special calculation function using atomic coordinate data can be added by writing a new plug-in module. In contrast, macro language has been used in some systems, it

never be faster and powerful than a binary code of plug-in module. A robust module interface design is now revised.

Prototyping has completed on Unix with X-Window system. This first version has basic protein visualization features, such as several molecular model representation, rotation and two new features: 1) boundary outline to distinguish different molecules; 2) amino acid sequence windows are linked to 3-dimensional viewing window of the protein, where a selection echo is shown also in another window. It gives us a nice tracking view of peptide chains on navigating large proteins. Several examples of protein pictures made by this prototype will be presented in poster: a molecular interaction study of muscle proteins. Actin (45kD) and Myosin (head sub fragment S-1 : 120kD) which are known to interact to generate force. Actin forms a filament in muscle, so several Actin monomer should be drawn, and one or two Myosin would interact in a picture. This case will be more than 4000 of alpha-carbons.

Our program was written in C with Xlib and ordinary libraries and going to be released for Unix systems. Versions for personal computers are also planed to take advantage of their high potential in hardware.

References

[1] Namba,K., Caspar,D.L.D and Stubbs,G. "Enhancement and Simplification of Macromolecular Images.": *Biophys.J.* 53 (1988) 469-475.