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Simplifying the Science and Art of Molecular Dynamics

Using molecular dynamics (MD) software, scientists can simulate molecular movement to study biological phenomena that currently cannot be observed experimentally.

But the value of MD software can be outweighed by its steep learning curve. For example, to run GROMACS, a popular MD software package with a 300-page user manual, users typically deal with four different programs—each with at least 15 different options that are run via a com-

putational biologist and programmer for Simbios.

OpenMM Zephyr is built on a version of GROMACS that incorporates the OpenMM libraries (see Summer 2008 issue), enabling it to run on graphical processing units and making it possible to run larger and/or longer simulations than can be run on CPUs. But Zephyr only exposes a tiny fraction of the numerous GROMACS parameters—often via pull-down menus—narrowing the choices so that a user can quickly get a simulation running. Zephyr is also integrated with the widely used molecular dynamics viewer VMD; simply selecting the checkbox for VMD launches it and displays the simulation as it is running.

Bruns points out that although OpenMM Zephyr is easy to use, it is not a black box. “Complicated things are done by Zephyr and we don’t want the user to just be a monkey turning the crank,” says Bruns. OpenMM Zephyr is therefore designed around three guiding principles: discoverability—exposing information so that the user can drill deeper to understand what is going on; feedback—communicating to the user when things go wrong, as well as when things go right; and expert convention—building in the parameter choices, workflow, and other best practices of expert MD users to guide an individual.

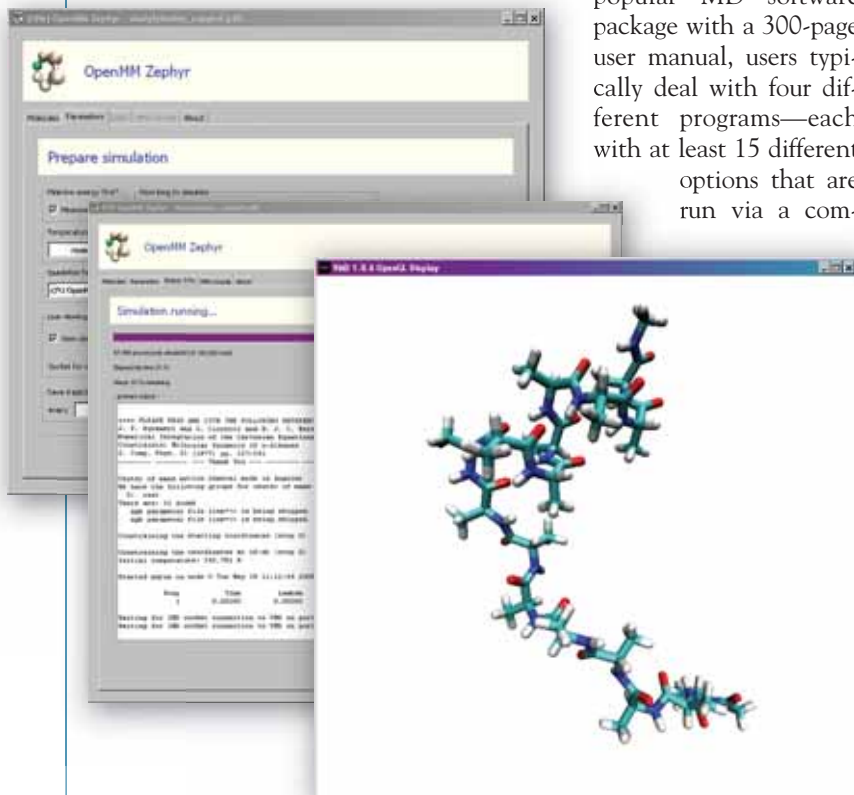
The approach seems to be working. “From a cost-benefit analysis, Zephyr is very attractive,” says **KC Huang, PhD**, an assistant professor in bioengineering at Stanford University. For people like him who aren’t well-versed in using MD on biological molecules, he says, OpenMM Zephyr is a great way to explore whether it will be helpful or not, without making a huge initial time investment in learning.

For **Victor Pinks, PhD**, the science chairman and technology director at Marmion Academy, a high school in Aurora, Illinois, Zephyr’s accessibility and ease-of-use were compelling reasons to switch to it. He and his student **Timothy Hagerty** had been designing laboratory exercises using another MD program. “When we saw OpenMM Zephyr, we thought, ‘That’s exactly what we want.’ Now we can go right into the science,” says Pinks.

Klaus Schulten, PhD, professor of physics at the University of Illinois at Urbana-Champaign, says, “Molecular dynamics is becoming more and more of a tool for use by biomedical scientists, including both clinical and experimental investigators. So it is really wonderful that Simbios is simplifying the science and art of it.” □

mand line interface. The first hurdle though is getting through the multi-step installation process. And other MD packages are just as complicated. Installing and learning to use any of them can be daunting. To address that problem, Simbios has just released a new version of OpenMM Zephyr, an application to simplify the MD process. It has a one-click installation process and provides a graphical user interface that guides an individual through the workflow for setting up, running, and viewing an MD simulation.

“With OpenMM Zephyr, we’ve created a software that is a good educational tool for learning how to use molecular dynamics. It also makes it more comfortable for even an expert user to get things done quickly,” says **Christopher Bruns, PhD**,



DETAILS: OpenMM Zephyr can be freely downloaded from <http://simtk.org/home/zephyr>. It currently runs on Windows and Macintosh platforms. The Linux version is expected to be released later this year.

