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COMPUTER SOFTWARE REVIEWS

Mathematica 6.0. Wolfram Research, Inc., 100 Trade Center Drive, Champaign, IL 61820-7237. www.wolfram.com. See Web site for pricing information.

Mathematica is an outstanding piece of software for both analytical and numerical calculations and is a valuable tool for research in chemistry and in the classroom. This latest version has some significant improvements over its predecessor. Specifically, Wolfram Research, Inc. has added new functionality to the program, such as dynamic variables and interactivity, and has also improved the interface, which will make it easier for new users and students to debug their notebooks. This release marks the company's 20th anniversary, and they accurately describe it as a major step forward.

A strength of Mathematica is the ease with which complicated calculations can be performed and the results visualized. This is particularly true of symbolic calculations, for which it is almost unrivaled in terms of functionality. Mathematica can handle numerical calculations and can even be used as a programming language for numerical simulations, but it is not quite as natural in this regard as some other environments such as Matlab, or open-source options such as R, C, or Fortran. Input and output of data have been improved in this version, but it is really the large collection of numerical algorithms built into Mathematica and the graphical environment that make it so useful for research chemists and students.

One of the major improvements in the sixth edition is the new interactive functionality. One simple example is the viewing of 3D structures. In past versions, the view could only be changed by manually editing the ViewPoint variables in the 3D plotting functions. It is now possible to rotate 3D objects with the mouse. It could be argued that this should have been implemented in earlier releases, but at least it has been added to this version. Another improvement is the capability to add comments or change the properties of vector objects in output graphics, which when combined with improved exporting of graphics, such as in the pdf format, will make it easier to produce figures for scientific publication.

A more significant advance is the ability to generate plots with dynamic variables. This is a clever idea in which plotting and numerical functions can be called through a Manipulate wrapper function. Manipulate specifies a set of variables that can be dynamically changed with sliders or toggle buttons. The resulting plot or function can then be adjusted by changing the dynamic variables with the mouse. This will be particularly good for demonstrations in the classroom, where is it often helpful to show how a function or model changes with different parameters. This dynamic interactivity extends the functionality of Mathematica into the realm of graphical programming and may even compete with java applets as a tool for presenting small graphical scientific simulations.

Another improvement is that the values of dynamic variables are updated whenever commands are executed. In previous versions of Mathematica, commands influence the state of the kernel and present their output strictly in the order that they are executed. This can be confusing to students as they go back and forth in a notebook or if the kernel becomes left in an unexpected state; many get into the habit of killing the kernel at regular intervals to see if it will fix their problems. It is not clear if dynamic variables will make this more or less confusing, but it is good to have the option of generating variables and expressions which remain consistent with the state of the kernel.

There are also a few areas that have been reworked in this new version of Mathematica to reduce the frustration of new users. Input commands are now colored dynamically to illustrate how Mathematica is parsing them. This is very well done, so that common syntax errors, such as missing or incorrect brackets, become obvious. Error messages have been made more intelligible, often describing the problem more clearly and suggesting a solution. The help functions have now been unified into a documentation center that is easier to navigate than in previous versions.

One last feature, which could be of interest to chemists, is the large collection of integrated data sources that are automatically available from Wolfram's servers. One package in particular, ChemicalData, has a large list of chemical compounds along with their structures and a collection of physical properties for each. Basic two-dimensional structural diagrams are available, as well as three-dimensional molecular structures that can be viewed and rotated. This is a neat new direction for the program, allowing it to provide current information specific to a group of users in a field such as chemistry.

Some users may want to wait before upgrading from Version 5 to 6; there are still many reported bugs and incompatibilities with notebooks created from previous versions. Version 6 also unfortunately does not allow exporting to Version 5, which in turn is not consistently able to load a notebook created with the current version.

Overall, Mathematica 6 has many new features and improvements that make it a worthwhile upgrade. Wolfram Research is clearly continuing to innovate and redesign this product. Their improvements in basic functionality—and academic pricing—will continue to make this a good choice for the classroom. It is also very nice to see that they have kept chemists in mind as they add new features.

Graeme Henkelman, *University of Texas at Austin*