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COMPUTER SOFTWARE REVIEWS

Mathematica 7.0. Wolfram Research, Inc., 100 Trade Center Drive, Champaign, IL 61820-7237. http://www.wolfram.com. See Web site for pricing information.

Wolfram Research released Version 7.0 of *Mathematica* in the fall of 2008, which promises faster computation, better accessibility, parallel computing capability, image processing, and the extensive ability to plot bar and pie graphs. In my personal experience, one of the key strengths of this software is the ability to work with mathematical expressions far outside of what is feasible on paper. Combined with the program's ability to handle and parse binary and ASCII data within a reasonably simple programming environment, this makes the software a well-rounded platform for analysis and modeling of experimental data. With the new version, Wolfram Research promises a one-stop mathematical "Swiss army knife".

For the new user, learning the software can be a rather intimidating task. The program offers thousands of functions that can be used in a variety of syntactical constructs. Although the user interface within the program, i.e., the notebook, can be formatted as a text file, the interface is in principle in command-line form. As with other programming languages, the interface does not allow the user much room for spelling or punctuation mistakes, and error messages are often numerous and hard to decipher.

The user interface in Version 7.0 has been improved significantly from the earlier version (5.2) that I had integrated into my physical chemistry course. Access to help files and tutorials has been greatly improved, reducing the steepness of the learning curve at no cost to the content or to the ability of the program to handle complex algebra and data. The most useful tools here are the documentation center, which gives reference-style access to functions and operations, and the function navigator, where examples and descriptions of the syntax in the program are found. The documentation provides scope, general applications, and examples of possible issues with using the function. For those going deeper into the underlying program, an electronic version of the *Mathematica* book can be accessed within the program. The *Mathematica* book offers tutorials of the most common functions in the program. The user interface also includes code-coloring, a feature that many programming editors have included for a long time, as well as better color schemes in graphs, scatter plots, and surface plots in this version than in previous ones.

I find these improvements alone compelling enough reason for investing in Version 7.0. Although the initial learning curve has certainly been made easier, several common functions could use better help files and examples. In particular, import, export, and basic procedural programming, such as loop constructs and conditional tests could be better explained for beginning users. All of these are important when employing the program in data analysis and modeling.

Several neat features appear in Version 7.0 that are truly new to the program. The new family of dynamic functions significantly changes the previously command-line-like notebook interface and allows integration of sliders, touch pads,

and game controllers. These additions employ the syntax that is used throughout *Mathematica*, so proficiency and integration are quick for those that are familiar with the basic use of the program. Here again, the help files in the virtual book are well written and accessible. The dynamic interactivity allows users to demonstrate the behavior of mathematical functions, calculated objects, and extract instances from large data sets easily. The interactive addition also offers a packaged "Manipulate[]" function, where the software combines variable manipulation into a object that can then be exported into a stand-alone player item. Some useful demonstrations relevant to chemistry using this can be found at the Wolfram Research Web site: www.demonstrations.wolfram.com.

Mathematica 7.0 also introduces a processing capability for images. Here the software does what many other programs offer; however, the strength here is that the images, as well as the manipulation of the output, can be tied to a mathematical evaluation; i.e., the hue or size of an image can be varied according to a value calculated elsewhere. In my test of manipulating AFM images, I found the syntactical numerology daunting, although eventually the outcome was acceptable. It appears to me that Wolfram is attempting to "wow" its customers with visual images by adding the image processing feature, rather than sticking to the highly analytical realm that has been the breadwinner so far. I had similar feelings with regard to the extensive array of pseudo 3D-pie, 3D-bubble, 3D-rectangle, and 3D-sector diagrams, where the focus is again on visual pleasure. Admittedly, the output graphics have a clean look to them as long as the data are simple, but variation outside the default settings requires extensive selection of "magic numbers" and keywords.

Version 7.0 also updates the "extended chemical data", which I found to be disappointing in comparison with the other improvements in the program and cursed with being too broad and too shallow as a result. The database has computable information for several tens of thousands of chemicals, which includes information about safety, physical, thermal, and structural properties. I found it annoying that there was little or no consistency in units, unless you figure out how to type the correct keyword into the extraction string. I have a similar gripe with regard to the physical conditions that apply. The values given for boiling points, density, and refractive index were not always accurate and were often not provided. Besides structural data and atom coordinates, I found little useful information that is not readily accessible elsewhere. My feeling are that this new addition may be useful to some researchers but few of those will be chemists.

In summary, the newest version of *Mathematica* 7.0 has substantial and important improvements in the user interface and help documentation. This will shorten the time new users need to become proficient in the basic applications and will significantly help integrate the program into research and teaching programs. The program remains a well-rounded and very powerful mathematical platform, where analytical functions, numerical data, and programming can be combined. Minor programming skills are needed to expand the use of

the program to data analysis and simulations. The new version has a nifty dynamic interactivity, which allows live update of the contents of the entire notebook by changing the designated interactive variables, and it is simple to use. Many additions to the program focus on graphical presentations rather than improving the analytical value. These additions gave clean-looking default graphics but were often cumbersome to modify and are unlikely to become a compelling reason for purchasing the program.

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