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Computer Software Review

Mathematica 5.1 Wolfram Research Inc., 100 Trade Center Drive, Champaign, IL 61820-7237. www.wolfram. com. Suggested retail price: $1880 (U.S. and Canada) includes one year of premier service. Academic price: $895. Student version: $139.95.

Dmitrii E. Makarov

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Mathematica has a well-established reputation as an integrated environment for technical computation that combines powerful data analysis, symbolic manipulation, numerical computation, and graphical capabilities in a single package. This software incorporates knowledge from many mathematical handbooks and can solve differential equations, do integrals (numerically or analytically), expand functions in Taylor series, simplify algebraic formulas, multiply and invert matrices, fit numerical data with analytic functions, and perform fast Fourier transforms, to mention just a few of its capabilities. It also includes powerful tools for statistical data analysis and is a comprehensive computer language, allowing the user to write sophisticated codes that can take advantage of the built-in algorithms and routines. Mathematica provides comprehensive visualization tools and allows users to create interactive presentations that can be used for educational purposes.

While Mathematica is designed to be a self-sufficient, do-it-all package, many users will appreciate that version 5.1 includes many additional importing and exporting file formats, making it easy to use Mathematica in conjunction with Excel, Tex, Matlab, and other programs or to produce .avi movies that can be included in PowerPoint presentations. In addition, Mathematica now allows importing of data directly from many Web sites. Other new features in this latest release include a built-in extensible GUI kit that allows users to create customized graphical interfaces, new graphic capabilities, a benchmarking tool, and a number of algorithmic enhancements that further improve the program's performance.

A fairly substantial investment of time may initially be required for a first-time user to fully learn Mathematica's unprecedented capabilities. Several features, however, facilitate this learning process. A 10-minute interactive tutorial can be accessed from Mathematica to introduce the basic capabilities of the software. *The Mathematica Book* by Mathematica's creator Stephen Wolfram is directly accessible from within the program's Help browser. In addition, the package comes with two booklets, *A Quick Tour of Mathematica 5* and *Getting Started with Mathematica 5.1*, that guide the user through the installation process, explain how to use the program, and review its basic features and capabilities.

Several standard packages included in the software provide convenient access to data of relevance to specific chemical applications. For example, the package "ChemicalElements" contains basic information about chemical elements, their electronic structure, and physical properties, and a database containing resonance absorption lines may be accessed through the package "ResonanceAbsorptionLines". The values of fundamental constants can be easily accessed via the "Physical-Constants" package, and another package, "Units", performs conversions of units. More importantly, the numerical computation, programming, and data analysis tools provided by this software are suitable for a wide range of chemical applications, both industrial and academic, and Mathematica's capabilities for visualization make it highly suitable as an interactive tool in chemical education.

Dmitrii E. Makarov,
University of Texas at Austin