TECHVIEW
SOFTWARE

A Mathematical Swiss Army Knife

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It is hard to imagine a scientific software tool that is equally useful to a math professor, a cardiologist, a protein chemist, a population biologist, a civil engineer, an architect, and an atmospheric scientist. Mathematica is just such a program. Released on 23 June 1988, Mathematica 1.0 garnered immediate acclaim for its unique approach to computer-based mathematics. With a powerful programming language and a dizzying array of functions, the program can be adapted to perform diverse calculations for almost any scientific need. Some of these include performing statistical analyses, drawing graphs, deriving mathematical proofs, modeling natural processes, and even making nucleic acid sequence comparisons. Among the enhancements in this new version are an increased calculating speed and efficiency, improved import-export capabilities, spell checking in the notebook interface, and over 100 new or enhanced mathematical functions. In addition to the basic program, modules are available that extend its utility still further. The modules provide diverse capabilities, from wavelet and economic analysis to amateur astronomy, as well as a variety of technical publishing tools.

Mathematica 4.0
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The latest version of the program comes with three manuals: a very thin *Getting Started with Mathematica*, the *Mathematica 4 Standard Add-On Packages* manual, and the huge *The Mathematica Book*. For the first-time user, reading the *Getting Started* manual will be an excellent time investment. It contains brief sections on starting the program, using the online help, using the palettes (onscreen tools users click on to use), understanding the mathematical notation specific to the program, and using the program's simple calculations. It introduces many of the terms with which novices need to become familiar and assists them in solving problems quickly with either the Mathematica programming language or the palettes. The *Add-On* manual is a concise description of the standard packages that are included with version 4 which extend the functionality of Mathematica into areas such as algebra, geometry, linear algebra, number theory, and statistics. Specific commands in each section are documented and their functions are described with examples.

For those who want some heavy-duty reading, *The Mathematica Book* is a 1470-page reference that introduces the enthusiast to a brief coverage of most of Mathematica's capabilities as well as a wealth of background material. The book discusses the innumerable built-in functions of the program with illustrative examples. For help with specific problems, Mathematica offers extensive help menus, an online FAQ (frequently asked questions) area at its World Wide Web site, and an excellent technical service staff. For users that need further assistance, texts such as *Mathematica by Example* are available (*1*). Over 250 books in 14 languages have been published on Mathematica to date.

Mathematica runs on a variety of platforms, including Windows 95, 98, or NT; Macintosh; Linux; SunOS/Solaris; and several others. The program uses about 150 MB of hard disk space, but it can also be run from a CD-ROM, in which case one needs only a little over 40 MB to run the program. Though a computer with an old 386 processor is the minimum system listed in the *Getting Started* manual, it is rather impractical to attempt to use the program in such an environment. A more realistic system includes a Pentium processor for Windows (PowerPC for Macintosh), 32 MB of RAM, and an SVGA monitor. The latter is particularly important if the program is used extensively for making graphic images.

The latest version of Mathematica will import standard Lotus and Excel files but can also handle both resolution-dependent and -independent graphics such as GIF, EPS, JPEG, AU, WAV, HDF, and others. Basically, all of the action with respect to data management occurs in the program's cells and notebooks. The cell is Mathematica's basic unit of workspace and appears anywhere in the blank workspace where the pointer becomes an I beam. When the mouse is clicked during this mode, an insertion bar appears and the user may begin typing. By default, the new cells are input cells and either text or mathematical notation may be entered. Collections of text, graphic, hyperlink, and mathematical cells on a given topic are saved as notebooks. These notebook documents can even include animations and sound. A document of this kind can easily be shared with co-workers, regardless of the kinds of computers they have because the documents are completely platform-independent. In fact, one does not even need Mathematica: MathReader is a free utility that permits anyone to read the document.

Another useful feature is that Mathematica will create an HTML version of any of its notebook documents with the use of a single menu command. This feature is invaluable for users who would like to post their notebooks on the Web. The ability to easily import or export data and graphics and to export to HTML/MathML (an HTML extension specially designed for describing mathematical expressions) makes it easy for users to integrate Mathematica with other tools they may be using. Documents produced in the program can readily be published in a variety of formats, whether presentations or technical reports. A very attractive feature in this regard is the availability of publication-quality typeset mathematics. Mathematica can automatically translate a document into a TeX input file (a technical typesetting system and macro language used to create typeset output from ASCII documents that contain text and descriptions of mathematical expressions).

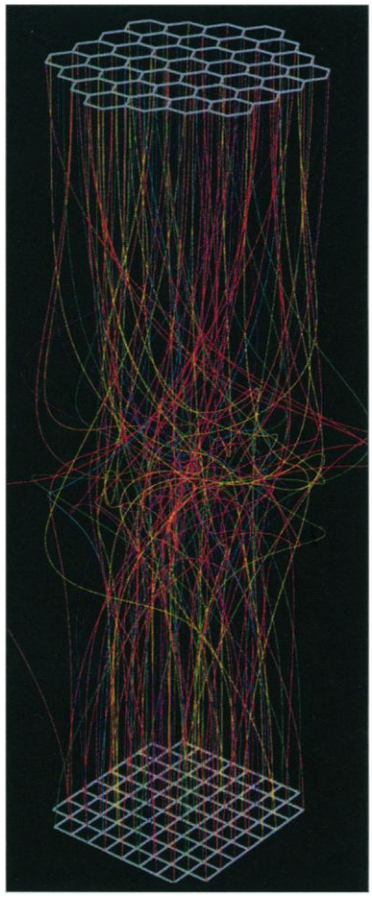

Fig. 1. Random smooth interpolation from a hexagonal to a square lattice. Zeroes of the generalized Riemann zeta function $\zeta(a, s)$ as a function of both

Beginning with version 3, Mathematica incorporated several palettes that make life considerably easier. The palettes, while covering only a small minority of Mathematica's functions, assist with the most frequently used

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commands. At the touch of a button, a palette will display a function that a user may employ for either symbolic calculations or numeric calculations over a specified range. The core palettes cover the following areas: basic arithmetic, algebra, polynomial manipulation or simplification, complex numbers, matrix operations, trigonometric functions, calculus, integer and special functions, and graphics, as well as special symbols and Greek letters. The use of these palettes can greatly simplify many calculations. Two other palettes that come with the program are of particular interest to scientists: the periodic table of the elements and physical constants. These permit input of various kinds of chemical and physical information.

Mathematica's capabilities extend far beyond its palettes, and it has a plethora of in-depth utilities that cannot be adequately described in a short review. For example, intermediate calculations can be entered on either side of an equal sign, and if they are equivalent, a "true" will be returned. In this fashion, the program can help both expert and student step through either proofs or the most tedious of calculations. For other problems, complex terminology can be shortened and recast in terms of other variables, all of which are easily presented to Mathematica in familiar language. Many times an unexpected answer may be returned, especially from an integral or derivative expression. In these cases, built-in functions such as Expand, Simplify, and Factor are invaluable. As an example, the following simplifies Sqrt[x^2] under the assumption that x is an element of the set of real numbers:

```
Simplify [Sqrt[x^2], x \[Element] Reals]
```

This simplifies to Abs[x].

As another example, Simplify [Sqrt[x y] <= x + y/2, x >= 0 \[And] y >= 0] evaluates to true, which "proves" that the geometric mean is always <= the arithmetic mean with the assumption that both numbers are positive.

Mathematica thus also makes an excellent teaching tool, by helping the student to more easily comprehend complex analytic manipulations.

The sum total of Mathematica's capabilities is overwhelming, but a few features suffer from lack of development. In standard statistical programs, such as SAS, JMP, SPSS, and STATISTICA, the user expects to push a few buttons or to type minimal code to generate many lines of output, including descriptive statistics and diagnostics. In the statistical module of Mathematica, however, obtaining all of this output is cumbersome. There are many small problems, mainly with the code, that mostly affect the uninitiated. It is still a minor irritation to navigate Mathematica's jungle of curly braces and brackets. The ":=" (for a definition) and "==" (for "equals") also take a bit of getting used to, and the program's case sensitivity will drive some to distraction. There are valid programming reasons for these items, however, and those new to the program usually become acclimated rapidly.

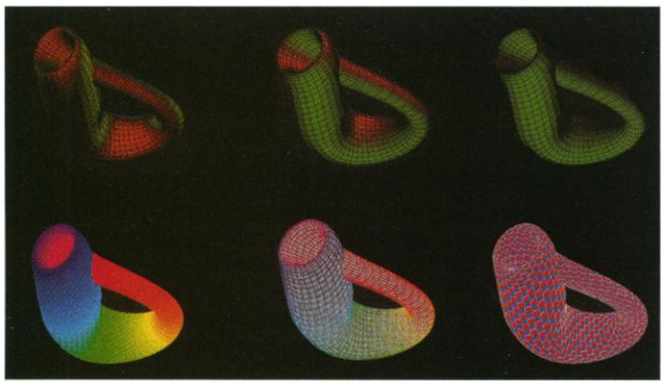

Fig. 2. Representation of a Klein bottle, showing the effects of varying light-source position, color, and surface color.

Mathematica is both a mathematical program and a programming language, and as such it generates numeric analyses. The program also has graphic capabilities, although this statement is akin to saying that Picasso could sketch a little. Numerous examples of beautiful graphic images produced with Mathematica can be found in the books referenced at the end of this article (*2*). From simple two-dimensional lines to the most intricate, colored, complex surfaces, Mathematica will rarely disappoint (Fig. 1). As is usually the case with programmed graphics, code can be endlessly recycled and enhanced. Any function can rapidly be visualized with the plot function by merely adding ranges for named variables. These images can be customized just as quickly with color, dashes, aspect ratios (relative orizontal and vertical sizes), and labeling of axes. In addition, the Viewpoint option can be enhanced with the three-dimensional Viewpoint Selector. This will allow clicking and dragging to change the perspective instantly. Stunning effects may be achieved with the shading and lighting options (Fig. 2). For the mathematically inclined, contour plots can be used to investigate the behavior of many functions at critical points. These graphics functions are so extensive that users are limited only by their imaginations.

As an interactive calculation tool and a high-level programming language, Mathematica is an extremely powerful tool with which to understand and solve a variety of problems. Any difficulties inflicted upon the novice by the stiff programming language are more than compensated for by the sheer number of functions and the flexibility of the program. The versatility of Mathematica in modeling and simulation studies is evident from a visit to Wolfram Research's Web site, where the company has posted a section entitled Users' Experiences (www.wolfram.com/solutions/biomed/how.html and www.wolfram.com/solutions/highered/how/). These pages contain descriptions from scientists and engineers in many fields who have used Mathematica in their work. The program has been used for everything from running echocardiography systems to predicting protein structure from amino acid sequence, from analyzing bee behavior to designing seismic retrofits for the Bay Bridge, and from figuring the probability of engine failure during a space launch to assisting in architectural design.

As for the improvements in the latest version of Mathematica, the makers of the program point to significant increases in computing speed. One example is the new algorithm used for Fourier transforms, where a matrix of 250,000 random elements is transformed in about two seconds. Not only is version 4 faster, it requires less memory to carry out the calculation than the earlier version did. Possibly of less practical use to most users, but illustrative of the program's mind-boggling computational prowess, is the ability of Mathematica to calculate the value of π to the millionth place in a matter of minutes.

Wolfram Research has done everyone a favor by forgoing the numerous expensive add-ons and yearly upgrade fees that are so popular with many companies. To add to the program's attractiveness and usability, the company offers a technical support telephone line, several foreign language editions of both the manuals and the program, a user-friendly Web site, and up-to-the-minute access to the latest news. It was disappointing to see the company abandon the training classes for using Mathematica that were offered on the Champaign campus, but these have been replaced by courses taught off-site by several third-party vendors. The Mathematica World Conference and the periodic developers' conferences do much to extend the enthusiasm for this product. I would urge any interested analyst to contact the company for a demonstration disk.

References

1. M. L. Abell and J. P. Braselton, *Mathematica by Example*, (Academic Press, San Diego, ed. 2, 1997).
2. *Graphica 1: The World of Mathematica Graphics. The Imaginary Made Real: The Art of Michael Trott*, J. Bonadies, Ed. (Wolfram Media, Champaign, IL, 1999); *Graphica 2: The World of Mathematica Graphics. The Pattern of Beauty: The Art of Igor Bakshee*, J. Bonadies, Ed. (Wolfram Media, Champaign, IL, 1999).