COMPUTER SOFTWARE REVIEWS

Mathematica

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Mathematica[1] is a large, sophisticated software system that can perform numerical and symbolic mathematical computations and produce sophisticated graphics. The system is used by people with various needs and backgrounds ranging from students to engineers, scientists, and researchers. The number of alternative uses for the software is virtually unbounded, and this review will try to point out some highlights and useful features. The review will point out the types of operations supported with some specific examples, but it is not possible to be exhaustive in coverage. The tests reported here were run on a 25-MHz MS-DOS 386 machine with a 4 MB RAM, a coprocessor chip, and color monitor, and using the appropriate version of Mathematica for this system.

When you buy Mathematica you get a shrink-wrapped package that contains the software along with documentation. The main document is a very nicely produced hardcover book from Addison-Wesley authored by Stephen Wolfram. It is now in its second edition and compares favorably in quality with standard college-level textbooks. A paperback book titled *Guide to Standard Mathematica Packages* is included. Some technical reports and other ancillary information are also provided. The *User's Guide* is the first document used in loading the software.

To run MS-DOS 386 Mathematica you need an Intel 80386, 80486, or compatible machine with 20, 25, or 33 MHz CPU clock speed and MS-DOS Version 3.0 or higher. At least 640 KB of conventional RAM and 3 MB of extended memory are required. At least 10–12 MB of free hard-disk space are needed to store Mathematica program files, and an additional 16 MB are needed for virtual memory swap areas.

Mathematica is available for a windows environment on 386-based machines, but it is a different version. The system is also available for a wide variety of other hardware platforms including machines from Macintosh, 386-based systems, Convex, Data General, Digital Equipment, Hewlett-Packard Apollo, IBM RISC System/6000, MIPS, NeXT, Silicon Graphics, Sony, and Sun. Prices vary tremendously, depending on the hardware and the number of copies licensed.

The installation of Mathematica on my 386 MS-DOS machine was extremely simple. A *User's Guide* comes in the package, and its chapter on Installation Procedure was clear and worked perfectly. It is only necessary to load the three disks in sequence, and the software does the rest.

Just what is Mathematica? It is a software system and language that is designed for mathematical and related applications. The operations can be divided into three main classes: numerical computations, symbolic computations, and graphical display generation. It also has a built-in programming language. Mathematica can work like a calculator to perform numerical calculations. It can handle numbers to any precision specified. It contains a very large collection of higher mathematical functions. Numerical computations can also be done with matrices, and sets of data can be analyzed. Mathematica can perform symbolic computations, for example, those involving the manipulation of algebraic formulas. It can solve polynomial equations and systems of equations. It can perform calculus operations such as evaluation of derivatives and integrals symbolically, and it can find symbolic solutions to ordinary differential equations. Mathematica can produce two- and three-dimensional graphics and also contour plots and density plots. Either functions or lists of data can be plotted. Great control of the graphical output is provided. Mathematica also includes a programming language which allows the user to build extensions to the basic system.

Learning how to use Mathematica: The system is very large, very capable, and quite intimidating at first. A reasonable beginning is to work through some of the explicit examples in the *User's Guide* and the book. This straightforward exercise can consume many hours, even if you are selective about which options to test. To go beyond running such examples requires some work on the part of the user. It is absolutely necessary to go back and forth from the screen to the book to look things up and test how they work with your own problem. Having the book at your side is essential while working with Mathematica. When you want to do a particular task and you don't know how, then it is essential to have access to more knowledgeable users, that is, someone to answer questions.

A very convenient feature of the software, which makes input manipulations much easier, is the ability to scroll through a session, edit previous input and run it again, and recall and edit previous input lines. Thus, when a syntactic error is made in typing an input line, it can be easily corrected without entering the entire line again. A log file can be kept to store the entirety of a session for later use.

Some examples of users of Mathematica will illustrate the range of the system's capabilities. Mathematica can perform numerical computations, and it can do so with any specified precision. Given the command:

```
N[100∧0.5,20]
```

to calculate the square root of 100 to 20 significant figures, the system responds:

```
31.62277660168379
```

within a fraction of a second.

The system has a multitude of built-in functions. An example is a function named "Binomial" that computes the value for binomial coefficients:

$$\frac{m!}{m!(m-n)!}$$

To use this function to evaluate the number of ways 12 things can be selected from 20, you enter the command:

Binomial[20,12]

and the response is:

125970

Integration, both symbolic and numeric, is well supported. That typing the command:

Integrate[x ∧ n,x]

yields the correct result very quickly is not surprising. But the system deals equally well with the following integration:

Integrate[1/(1+x ∧ 6),x]

which yields a complicated symbolic result with five terms containing arctangent and logarithmic functions:

$$\frac{-\arctan[\text{sqrt }[3]-2x]}{6}+\frac{\arctan[x]}{3}+\frac{\arctan[\text{sqrt}[3]+2x]}{6}-\frac{\log[1-\text{sqrt}[3]x+x^2]}{4\text{sqrt}[3]}+\frac{\log[1+\text{sqrt}[3]x+x^2]}{4\text{sqrt}[3]}$$

To print out this same expression in Fortran form, one uses the following command:

FortranForm[%]

which yields the following output:

-ArcTan(Sqrt(3) – 2*x)/6 + ArcTan(x)/3 + ArcTan(Sqrt (3)+ 2*x)/6 – Log(1 – Sqrt(3)*x + x**2)/(4*Sqrt(3)) + Log(1 + Sqrt(3)*x + x**2)/(Sqrt(3))

This expression could be immediately incorporated into another program being developed outside of Mathematica.

The generation of simple, two-dimensional plots of functions is easy. To plot the hyperbolic tangent function over the range from –8 to 8 requires the following command:

Plot[Tanh[x],{x,–8,8}]

Such easy display of functions makes visualization much easier than trying to reason from the mathematical formulas. Altering the appearance of this plot only requires adding additional items to the command line. Such plot attributes as the presence of a frame, the presence of labels, the drawing of grid lines, etc. are all easily changed. A slight variation in this function gives essentially a step function:

Plot[(1.0+Tanh[2x])/2.0,{x,–8,8}]

The appearance of the resulting plot is shown in Figure 1. Products of simple functions can be generated and plotted for easy conceptualization. The product function $(x)\sin(x)$ is plotted over the interval from –22 to 22 with the command:

Plot[x Sin[x], {x,–22,22}]

and the resulting plot is shown in Figure 2.

Three dimensional plotting is also easy. The plots are produced as colored, shaded images on the screen. They can be manipulated easily to produce gray-scale laser printer plots. Products of trigonometric functions make attractive functions for three-dimensional plotting because of their undulating

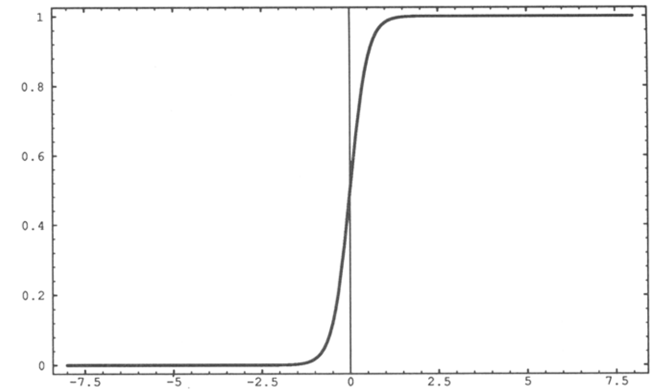

Figure 1.

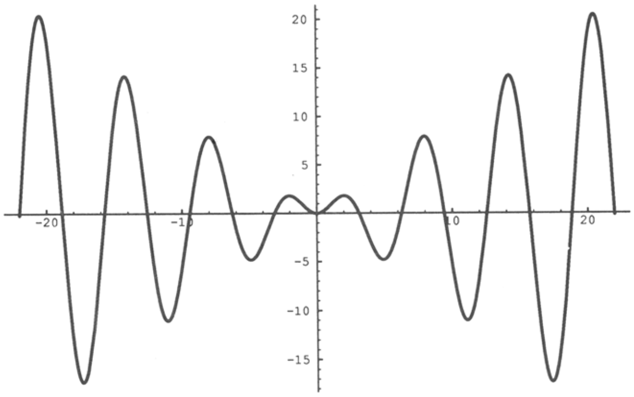

Figure 2.

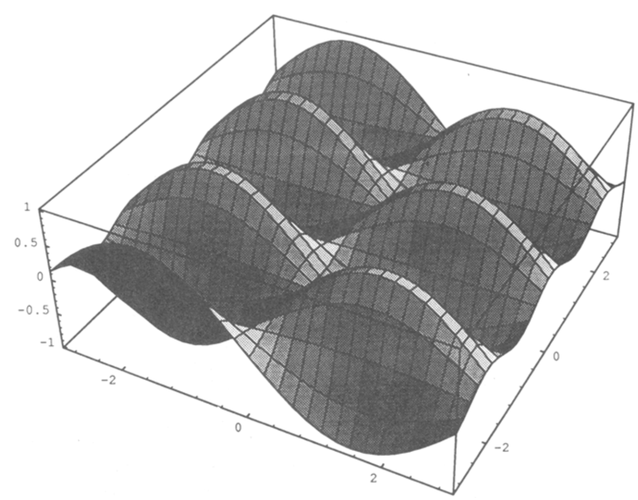

Figure 3.

surfaces. The following command:

Plot3D[Sin[x] Cos[3y], {x,–3,3},{y,–3,3}]

produces the plot shown as Figure 3. In addition to the usual attributes of the plot to be considered, the viewpoint can be changed from the default with an additional option on the command line.

Manipulating functions and getting quick visual confirmation of these effects on the appearance of a function is a strength of the system. A textbook example of the three-dimensional plotting routine is a simple Gaussian function:

$$e^{-(x^2+y^2}$$

which is plotted over the interval from –2 to 2 on each of the

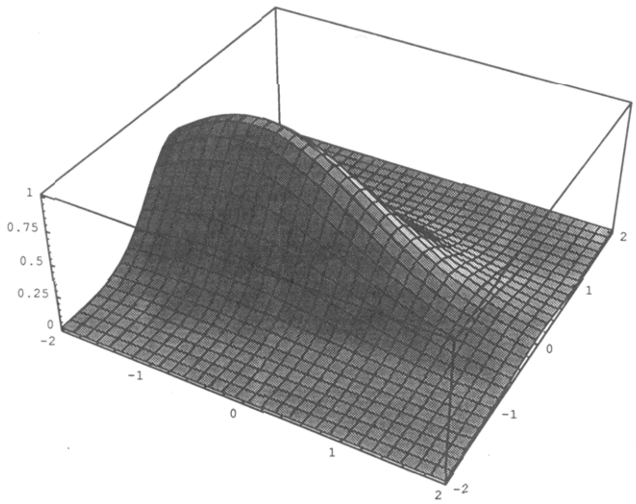

Figure 4.

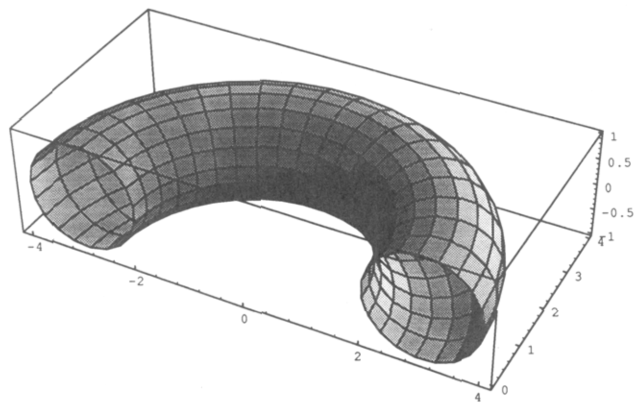

Figure 5.

two axes with the command:

Plot3D[Exp[-(x ∧ 2+y ∧ 2)],{x,-2,2},{y,-2,2}]

One can see the effects of introducing more parameters into the function to make it more general. Using values of $xm = -1$, $sx = 3$, $ym = 0$, and $sy = 0.5$ yielded the plot in Figure 4. Since in the function:

$$\exp\left[-\left\{\frac{(x - xm)^2}{sx} + \frac{(y - ym)^2}{sy}\right\}\right]$$

the term in x and the term in y are independent, the distribution is lined up with the two axes of the plot. Such a strategy could be used to visually check the appearance of a response surface during an optimization. Much more sophisticated three-dimensional surface plots can be generated from functions. An example is the generation of a complete torus with the command:

ParametricPlot3D[{Cos[t] (3+Cos[u]}, Sin[t] (3+Cos [u]}, Sin[u]}, {t,0,2Pi},{u,0,2Pi}]

By changing the range of the variable t to run from 0 to p radians, the half torus shown in Figure 5 is generated.

The core functions of Mathematica are extended with packages, which are routines written in the Mathematica language. The book *Guide to Standard Mathematica Packages* describes approximately 150 of them. Packages are provided in the following areas: algebra, calculus, discrete mathematics, geometry, graphics, linear algebra, number theory, numerical mathematics, statistics, miscellaneous, and others. The miscellaneous category includes a package named "Chemical Elements". This package contains information

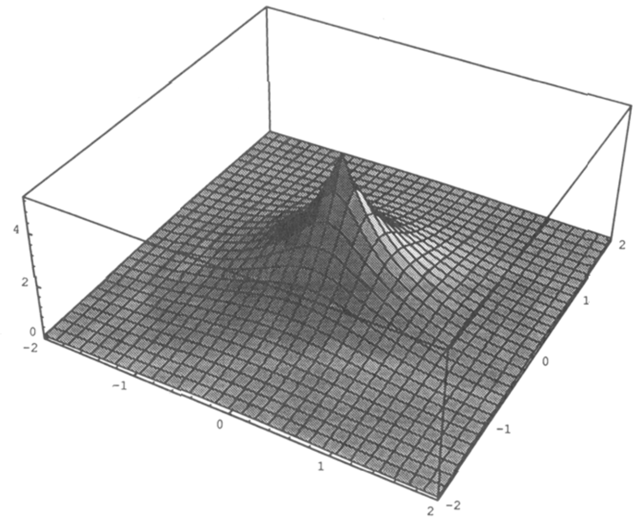

Figure 6.

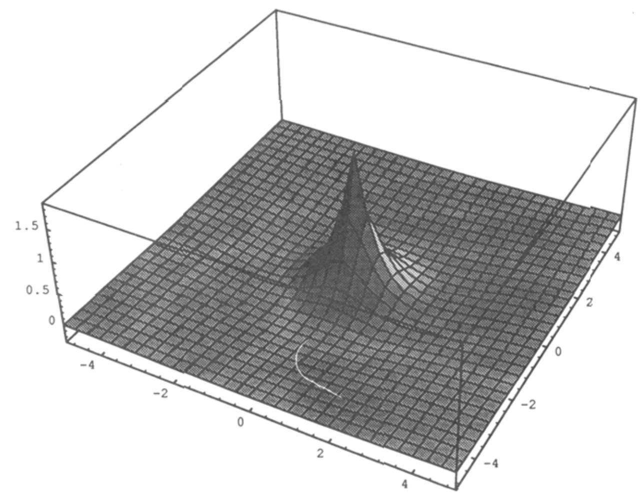

Figure 7.

about the atomic numbers, atomic weights, stable isotopes, melting points, boiling points, heats of fusion, heats of vaporization, densities, thermal conductivities, and electron configurations of the elements. A point plot of the atomic weights of all the elements can be generated with the command:

ListPlot[AtomicWeight[Elements]]

The electron configuration of an element is generated with the command:

ElectronConfigurationFormat[Gold]

Another package named "Polyhedra" can be used to generate three-dimensional plots of any of 10 common polyhedra from the cube and tetrahedron to much more complicated figures.

One chemically significant problem that suggests itself for a Mathematica application is the display of atomic orbitals. This topic has been addressed in a paper by Cooper and Casanova,[2] who described their development of a package called "Orbitals.m" for use with Mathematica version 1.1. In the following material, an abbreviated treatment is presented to show the possibilities of applying Mathematica to this task.

Following the nomenclature of Levine[3] for the radial factors in the hydrogenlike-atom wave functions, the 1s and the 2s atomic orbitals are represented by the following equations:

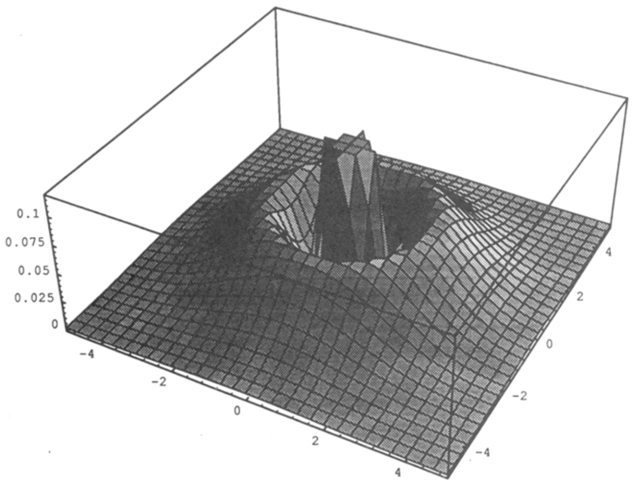

Figure 8.

$$R_{1s} = 2\left(\frac{Z}{a}\right)^{3/2} e^{-Zr/a}$$

$$R_{2s} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a}\right)^{3/2}\left(1 - \frac{Zr}{2a}\right)e^{-Zr/2a}$$

Figure 6 shows a three-dimensional plot of the 1s orbital, and Figure 7 shows a similar plot for the 2s orbital. The wave function dips somewhat below the zero plane in the 2s orbital, but it is not easily seen on this plot. Figure 8 shows a plot of the square of the 2s wave function with the z axis greatly expanded, and the rises and falls of the probability function are clearly seen. These types of plot (which are even more striking in color on the terminal screen) can be easily generated, thus providing the opportunity for visual interpretation of a function's meaning.

In summary: Mathematica is an extremely capable software system that can be used for many varied tasks in the general area of mathematics. Its strength lies in its ability to perform symbolic algebraic and other mathematical manipulations, coupled with the ability to provide graphical output. The package has capabilities in statistical analysis and general graphical production, but other packages can also do these tasks well. Mathematica is costly, and it requires a lot of memory and disk space to implement. It does take time to learn how to use the system, compared to other typical MS-DOS software packages. The input mechanism is somewhat cumbersome compared to other software packages. However, Mathematica shines where it can perform functions not easily available elsewhere that could be of great utility to chemists, especially in symbolic mathematics. The system couples with the outside world through its interfacing routines, and it can be used to tackle problems using its own language. Overall, Mathematica is a superior software product if its strengths match well with your needs.

REFERENCES AND NOTES

(1) Mathematica is available from Wolfram Research, Inc., 100 Trade Center Drive, Champaign, IL 61820-7237. The price varies widely depending on hardware platform and license specifics. The list price for single-user systems of the commercial and government version appropriate for a 386-based PC system under MS-DOS is $595 ($475 Educational) for the Standard version and $895 ($725 Educational) for the Enhanced version. The same prices apply to the Macintosh versions. For the Microsoft Windows version for 386-based PC systems, it is $995 ($795 Educational). Mathematica is available to students for $175 for MS-DOS, Microsoft Windows, and Macintosh machines.

(2) Cooper, R.; Casanova, J. Two-dimensional atomic and molecular orbital displays using Mathematica. *J. Chem. Educ.* **1991**, *68*, 487–488.

(3) Levine, I. *Quantum Chemistry*, 3rd ed.; Allyn and Bacon, Inc.: Boston, MA, 1983; p 121.

Edifice[1]

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This program is essentially a database manager with calculation and graphing capabilities. In its delivered form, it is a system for setting up to use the data from environmental methods of determination to produce a report. All output is based on user programming of the necessary algebra and selection of the graphing utility. The reports can be viewed, edited, and printed.

It is quite possible for anyone familiar with template creation for a spreadsheet database program to create the equivalent of this program in a relatively short time. While not a user-friendly environment, Edifice operates in a pulldown window format and allows methods and report formats to be saved and recalled depending on the input data type. The environment is very much like that of the early spreadsheets and word processors of the 1970s. Nothing about the operation is particularly intuitive, and a user community anticipating the MAC or Windows environment would be likely to be disappointed in that sense. Clearly this is a program for a conventional memory PC single-problem, single-user. Attempts to allocate sufficient resources to run Edifice in a Desqview environment were unsuccessful.

Certainly this program will serve to produce reports, and the user willing to work through the setup and testing could have a tool for report writing. The effort would be substantial on the part of the programmer. Perhaps a routine, Register method task manager in a service lab would find it useful.

REFERENCES AND NOTES

(1) Developed for Mittelhauser Corp. by Peter Jasim, 1991.