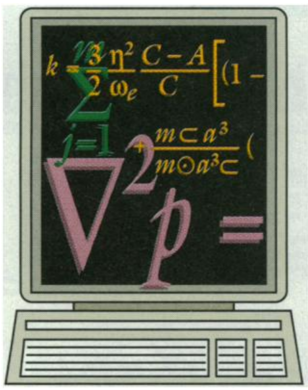
Bringing the Computer Revolution Down to a Personal Level

Super-fast computers that rip through hundreds of millions, or even billions, of calculations per second are changing science in a profound way, but a researcher doesn't have to have access to a supercomputer to get caught up in the computer revolution—personal computers will do just fine.

Already, computers have completely transformed the way that scientists communicate: Where once there was the telephone and mail service, and later the fax machine, now E-mail is the preferred mode for passing manuscripts and messages back and forth. And personal computers are dramatically changing other areas of the researcher's job as well. The machines are taking on the roles of technician and personal assistant, helping to perform experiments, gather and analyze data, perform calculations, and even prepare manuscripts and grant proposals. New software is changing the way science is taught. And databases offer quick and easy access to an exponentially increasing amount of information.

So as a service to our readers, *Science* surveyed the market to see what new products have turned out to be especially useful to scientists in a variety of different fields. The list of products mentioned below is by no means exhaustive, nor do we guarantee the quality of any of the products. Rather, the items are meant to be indicative of the types of tools that are becoming available and that researchers would like to know about. If you and your colleagues have discovered other especially valuable and broadly applicable products, drop us a line; they will be considered for next year's list—or perhaps for a short piece even before then. Consider the following pages a first effort to tip you off to computer products that might improve your working life in major ways.



Software for solving equations

From the beginning, computers were intended to crunch numbers—calculate pi to millions of places, multiply matrices with thousands of entries, or compute the position of a satellite hundreds of miles above the earth to within a few feet. But like a cleaning lady who doesn't do windows, computers didn't do symbolic calculations: algebra, calculus, or anything else in which equations are manipulated instead of numbers. Ask a computer to multiply two 1000-digit numbers: no problem. But don't ask it to calculate the derivative of sin x.

Richard Crandall, chief scientist for NeXT Computer Inc. and professor of science at Reed College in Portland, Oregon, puts it this way: Although number-crunching programs can give numerical answers to almost anything, they do only part of the job for scientists. They don't, for example, provide the insight into a problem that an equation can. In many cases, Crandall points out, the human mind learns more from answers expressed in "simple and elegant" equations than in the reams of numbers more natural to computers. The answer: symbolic mathematical software—it can actually prove a theorem or provide an exact solution to a problem, instead of giving an answer that is merely accurate to 5,10, or 100 decimal places.

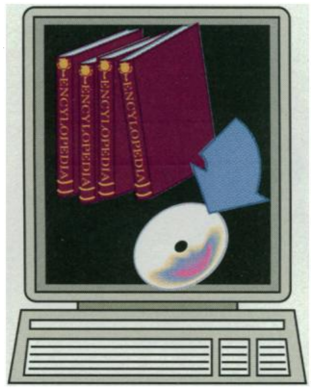
With the arrival of symbolic math programs, says Crandall, "the culture of science has changed, because now there are things you can solve that you couldn't before. We've been biased for 300 years in physics into solving [only] those problems that we can do on paper." But there are some problems, he notes, that are literally impossible to solve by hand—in general relativity, for instance, equations can run into the tens or even hundreds of pages. So in 1988, Wolfram Research Inc. in Champaign, Illinois, released **Mathematica**, a powerful equation-solving program for personal computers. That wasn't the first effort to respond to the need: Symbolic mathematical software has actually been around for more than a decade, but the early programs were designed for specialists—mathematicians and theoretical physicists who deal with large, messy equations on a regular basis and who had access to large, fast computers with big memories. **Mathematica** was the first powerful equation-solving software designed for personal computers, and since its release, a whole fleet of symbolic math software has run the rapids into the marketplace, promising to do for equation-solving what the hand-held calculator did for multiplication and division.

Symbolic math software also promises to change the way calculus and other math courses are taught. Rensselaer Polytechnic Institute in Troy, New York, for instance, has installed 500 computer workstations around campus as part of a program to teach calculus with the help of **Maple** (MathSoft, Inc., Cambridge, Massachusetts). With the software doing much of the messy, tedious manipulations of equations, the students are freed to learn the concepts behind the math, says Jack Wilson, director of Rensselaer's Anderson Center for Innovation in Undergraduate Education.

"What is it you want students to know how to do?" asks Wilson. In the good old days, students were taught, for example, how to take square roots by hand, but with calculators that's a skill that no one learns—and no one misses. Analogously, an instructor in a traditional calculus course may spend several days on trigonometric substitutions—a technique for solving integrals. "I never did trigonometric substitutions again in my life [after calculus class]," Wilson says. Rensselaer students learning calculus with **Maple** may not learn trigonometric substitutions quite as well as students in a traditional course, but they'll learn other things better, such as how to handle complex problems. Indeed, some students in the course complain that the use of computers just makes the course harder.

The symbolic math programs certainly make the course much closer to what the students will be doing in the real world, Wilson says. The scientists and engineers of the future will have not only calculators but also equation-solving software at their disposal. "If we can bring the educational world closer to the world they're going to experience, we'll be better off," Wilson says.

Several companies offer such programs, which usually do more than manipulate equations. Most of them also include numeric equation-solving capabilities and have graphics packages that display functions or solutions to equations as two- or three-dimensional graphs. Besides Mathematica and Maple, the programs include: **Axiom** (Numerical Algorithms Group, Philadelphia, Pennsylvania); **Derive** (Soft Warehouse, Honolulu, Hawaii); **Macsyma** (Symbolics Inc., Burlington, Massachusetts); **MATLAB** (The MathWorks Inc., South Natick, Massachusetts); **MathTensor** (MathSolutions Inc., Chapel Hill, North Carolina); **Microsoft MuMath** (Microsoft Corp., Redmond, Washington); **Polymath** (E&M Software Co., North Chelmsford, Massachusetts); and **Theorist**, (Prescience Corp., San Francisco, California).



Databases and CD-ROMs

The amount of information available to and generated by scientists has exploded in the past 20 years: genetic sequences, measurements of various properties of atoms, molecules, and materials, lists of astronomical objects, climate data, and on and on and on. And the flood is growing: the Human Genome Project and the Earth Observing System are just two of the projects that will generate more data over the next few years than scientists know what to do with.

It's not enough just to gather data—the information has to be put in an accessible form. That's where databases come in: Giant encyclopedias of electronic lore, they not only store copious amounts of data but come equipped with software systems that allow even casual users to find what they want quickly and easily. Today, with the help of a personal computer, any scientist can gain access to such encyclopedias, and the trend is toward making more and more data available on these databases—until at some point in the not-too-distant future, researchers will, with just a few keystrokes, be able to get their hands on almost any data they want.

Today, on-line services that give access to databases are so ubiquitous as to need little description. Several popular services allow researchers to reach dozens or hundreds of different databases with one phone call. One of the best-known among scientists is **STN International**, a collaboration among the American Chemical Society's Chemical Abstract Services, Fachinformationszentrum Chemie in Karlsruhe, Germany, and the Japanese Association for International Chemical Information in Tokyo. Its 120 databases cover all areas of science and medicine and offer a range of information: abstracts from hundreds of scientific journals, physical structures of millions of chemicals, and indexes of astronomical objects. It even offers the full texts of some two dozen journals, although the databases are not yet sophisticated enough to include the graphics accompanying the journal articles. (For an extended description of biological databases, see *Science*, 11 October 1991, p. 201.)

There are also services that offer much more specialized information, many of them run by government agencies. The National Institute of Standards and Technology (NIST), for example, has some 35 databases in its **Standard Reference Data** program, says program manager John Rumble, and the databases give researchers access to such information as the thermodynamic properties of refrigerants and the mass spectra of 53,994 different compounds. If a university library, a laboratory, or even a single researcher wants an individual copy of a database, that can often be arranged. NIST sells its databases on 3.5-inch diskettes at prices as low as several hundred dollars.

And some databases don't have to be called up on a researcher's personal computer—they are being installed directly into laboratory equipment to provide immediate comparisons between measurements and archived data. "They're becoming standard, for instance, on mass spectrometers," says NIST's Rumble. When a chemist runs a sample through a mass spectrometer, the resulting spectrum is as distinctive as a fingerprint, but the scientist still has to find its match from a collection of spectra of thousands of other chemicals. That used to be hard; now it's easy. With a spectrometry database and pattern-matching software built right into the machine, the mass spectrometer not only produces the fingerprint, it identifies the suspect. And a variety of other analytical equipment—such as diffractometers, which turn out crystal diffraction patterns, and nuclear magnetic resonance units—is being equipped in a similar way. "You get identification of compounds with just a few key strokes," Rumble says.

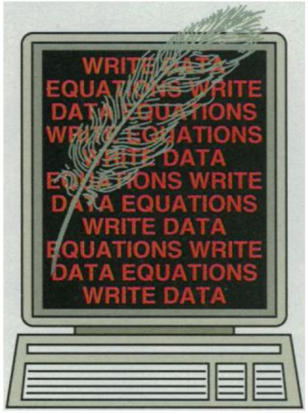
The biggest news in personal databases is a spillover from the stereo industry. Now that compact disks, or CDs, have taken over the music business from vinyl records, their next target is the personal computer, and they promise to break open the market for databases. In the computer industry, the compact disk is known as the CD-ROM (ROM standing for "read-only memory," which simply means that the user cannot record data onto the disk), but otherwise it's the same product—indeed some computer CD-ROM units can even double as CD players and play a little Vivaldi or Led Zeppelin when not being used to peruse Chemical Abstracts.

Although it takes more time to pull information from a CD-ROM than from a floppy disk, CD-ROMs hold a big advantage in the amount of information that they can store. Read by lasers instead of by the magnetic heads that read floppy disks, a CD-ROM can hold up to 600 megabytes of memory, or as much as 400 3.5-inch diskettes. That means that one CD-ROM can hold several databases, which normally take up anywhere from one to 20 diskettes each.

Since CD-ROM players for computers are still relatively new, the number of databases available for them is still limited, but more are released every week. At NIST, for example, only one or two of the 35 databases are on CD-ROM, but the institute expects that number to grow. STN has nothing so far, but it is considering putting some databases onto CD-ROM, spokesmen there say.

But if the major scientific organizations have been slow to move to CD-ROM, the same can't be said for commercial concerns. Dialog, a commercial database company in Palo Alto, California, has put three dozen of its 400 on-line databases onto CD-ROM, including a number of scientific databases in areas such as aerospace, chemistry and chemical engineering, materials science, electrical and electronic engineering, bioengineering and biotechnology, and medicine.

A number of other companies are moving into the CD-ROM field, putting various bibliographic or encyclopedic databases on compact disks. The following are a sampling of the many that have become available in just the past few months. **PatentView** (Research Publications, Woodbridge, Connecticut) contains copies of all patents issued by the U.S. Patent and Trademark Office, available within 2 weeks of the official release. **AIDS Information and Education Worldwide** (CD Resources, New York, New York) has 15,000 pages of material on AIDS collected from a variety of publications, and **AIDSLINE** (SilverPlatter Information Inc., Newton Lower Falls, Massachusetts) is a bibliographic listing of articles on AIDS from more than 3000 journals over the past decade. **General Science Index** (H.W. Wilson Co., Bronx, New York) indexes 109 English-language science periodicals in all areas, from 1984 to present; the same company also offers **Biographical and Agricultural Index**, a compendium of 226 periodicals. **Dissertations Abstracts Ondisc-B** (University Microfilms International, Ann Arbor, Michigan) contains abstracts of 600,000 Ph.D. dissertations in science and engineering from the United States and Britain. **SciTech Reference Plus** (R.R. Bowker, New Providence, New Jersey) has information about 125,000 scientists and engineers in the United States and Canada drawn from *American Men and Women of Science*, as well as data on scientific books and journals, and scientific research labs and companies in the United States. **Biotechnology Citation Index, Chemistry Citation Index,** and **Neuroscience Citation Index** (Institute for Scientific Information, Philadelphia) contain citations and abstracts from several hundred journals in each field, plus selected articles from journals not included in the citation index.



Software for scientific word processing

Only a decade ago, a researcher preparing a manuscript had no choice but to pull out the typewriter and hunt and peck through a paper, repairing mistakes with correction fluid and hoping that some new idea wouldn't make it necessary to type the whole thing over again. Does anyone remember the days when a single misspelled word might mean redoing a whole page? Or the implements for forming Greek letters or mathematical symbols—boxes full of individual plastic keys that could be inserted one at a time into the typewriter? Oh, and then there were carbon ring symbols, integration signs....

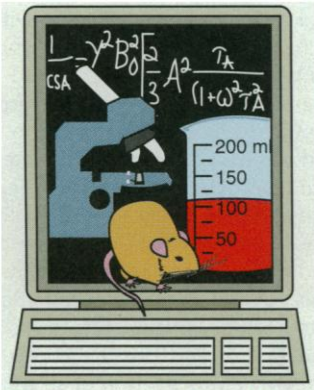
It all seems now like the Dark Ages. And if you haven't noticed, software makers are offering a burgeoning supply of products designed to make turning out a manuscript even easier than it already is.

Not sure how to spell *phthalylsulfathiazole* or *Pseudomonas flaccumfaciens*? You won't find those in the spell checkers that come packaged with WordPerfect or Microsoft Word, or even in your desktop Webster's. So it might pay to invest in a spell checker written for your particular specialty. Scientific Software in St. Louis, Missouri, for instance, offers **BioWords**, a biology spell checker for use with Microsoft Word 4.0 that includes 31,000 terms, as well as **ChemWords**, a chemistry package with 30,000 words.

Of course, word processing entails more than just words, and there is an abundance of software to prove it. **MathType** (Design Science Inc., Long Beach, California) is one of several programs that create mathematical formulas for insertion into text produced by a word processor. **ChemDraw** and **Chem3D** from Cambridge Scientific Computing Inc. (Cambridge, Massachusetts) are examples of software that draw molecular structures for inclusion into manuscripts. And **SigmaPlot** (Jandel Scientific, Corte Madera, California), **Graftool** (3-D Visions, Torrance, California), and **EasyPlot** (Spiral Software, Brookline, Massachusetts) are programs that create charts and graphs—a genus of software that contains dozens of species.

If a researcher doesn't want one program for word processing, another to write math equations, a third to draw chemical structures, and a fourth for graphs, there are ambitious software companies that package everything into one piece. **ChiWriter** (Horstmann Software Design Corp., San Jose, California) and **T**[3] (TCI Software Research, Las Cruces, New Mexico) are two of these "scientific word processors."

And to make putting together those 100-reference bibliographies as painless as possible, there are reference databases that do everything but read the articles for you. A representative example among the many in the field is **PAPYRUS** from Research Software Design in Portland, Oregon. It can keep track of up to 2 million reference citations, and once the manuscript is finished and you're ready to put the bibliography together, the program automatically creates it in any of several dozen prepackaged formats.



Software for teaching

Everyone who has ever taken a science or math course in college has a horror story to tell: math professors who write equations on the blackboard all class long without ever stopping to explain what they mean; biology teachers who fixate on classification and vocabulary to the point that students forget that something is alive under all that nomenclature; or physics instructors who focus on "laws" so much that the class seems like legal studies. While the new science-teaching software coming onto the market probably won't end all the horror stories, its proponents say it will make teaching easier and learning more likely.

Compare, for instance, the old and the new ways to teach physics students about vibrations, as described by Jack Wilson, director of the Anderson Center for Innovation in Undergraduate Education at Rensselaer Polytechnic Institute in Troy, New York. "In the old days, it was a very dry thing. You'd draw a sine function up on the board" and explain that it represented the motion of a spring or other physical object.

This semester, in several dozen U.S. colleges, students are instead trying out a multimedia computer system that brings oscillations and vibrations to life. As the computer screen displays the physical equations describing vibrations, the student can open up a window on the screen showing, for instance, Ella Fitzgerald hitting a high note that breaks a glass; the computer then presents an explanation of why the glass breaks. Or the student can watch a video of the famous collapse of Tacoma Narrows Bridge, when the suspension bridge began undulating as engineers were studying it and then oscillated more and more violently until it fell apart. The student can even stop the bridge video in mid-frame, trace a line along the curving bridge deck and then use another part of the software to mathematically analyze the curve and see that it is a sine wave.

The vibrations package is part of the CUPLE (Comprehensive Unified Physics Learning Environment) project sponsored by the American Association of Physics Teachers and directed by Wilson and physics professor Edward Redish of the University of Maryland. CUPLE's ambitious goal is nothing less than to change the way undergraduate physics is taught, by taking advantage of the inexpensive power of personal computers to help students visualize and analyze physical phenomena. The computers prompt students to ask more questions, Wilson says, pushing them to work more closely with both other students and the instructor. "It really ramps up the human-to-human interaction," and so, paradoxically, "the computer may be the thing that humanizes teaching."

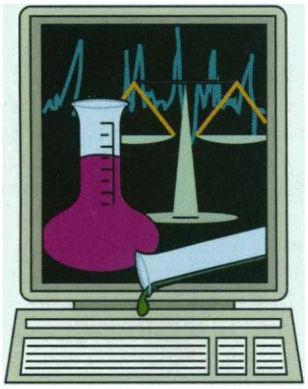
And not in just the physical sciences—even the life sciences are opening up to silicon instruction. Besides software anatomy programs for students too squeamish to dissect a frog or fetal pig, an increasing number of simulations and video-based instruction programs in biology are coming onto the market.

Simulations allow you "to do things you can't do without a computer," says Harold Modell, editor of *Computers in Life Science Education*. By adding a large-screen display, for instance, a lecturer can run a simulation of a biological system—gas transport in blood, say, or an ecology of predators and prey—and ask the students, "What do you want to do as a class [to alter the parameters in the simulation]? What do you expect to happen?" Then, Modell says, "you've turned this passive learning environment into an active learning environment. Now the instructor is a kind of colleague who is working with you against the computer. The whole psychology changes."

Simulation software seems particularly popular for chemistry courses, perhaps because that subject deals with many objects, such as molecules, that students will never see. Many molecular simulation programs exist, which allow students to see molecules on a computer screen, turn them, and even vibrate the molecules to watch how their bond lengths change, but that's just the beginning. **Ideal Gas**, produced at the University of Wisconsin Chemistry Department, simulates a tank filled with a gas—the student gets a feel for the ideal gas law by changing the temperature, pressure, volume, and amount of the gas and observing the effect on the piston that forms one end of the container. **Organic Reaction Mechanisms** (Falcon Software, Wentworth, New Hampshire) animates collisions and reactions between organic molecules. And **Atomic Orbitals**, also from Falcon Software, provides visualization of electron orbitals around atoms, with the goal of developing insight into bonding and chemical reactivity.

In the future, educational software for undergraduates will get better and cover more areas, to judge from a recent contest sponsored by *Computers in Physics* for innovative software in physics education. The winners spanned a range of subjects, from classical mechanics to chaos. David Trowbridge of Microsoft Corp. won with **EM Field**, a program that has students arrange electric charges or electric currents on a computer screen and then displays the resulting electric and magnetic fields; after enough experimentation, the student develops a feel for electromagnetic fields that's hard to obtain with pencil-and-paper calculations. Freeman Deutsch of the Harvard-Smithsonian Center for Astrophysics came up with **WaveMaker**, a program that teaches students about wave motion by letting them pluck a string and observe the resulting oscillations— all of it virtual action on a computer screen.

MacMotion, developed by Ronald Thornton of Tufts University, couples with microprocessor-based instruments to let students take data and analyze it automatically. An ultrasonic motion detector collects data from such experiments as the motion of a mass on the end of the spring, and the software automatically displays position, velocity, and acceleration. And no group of physics software would be complete without a chaos/fractals program, which every programmer seems to try his hand at sooner or later; the contest winner was **Mapper**, created by James Harold, a graduate student in the Laboratory of Plasma Research at the University of Maryland. Mapper leads the student by the hand on a tour of chaos-producing functions and produces the obligatory intricate and beautiful pictures of chaos.



Software for analytical chemistry

Many of the analytical instruments used in chemistry today are already so computerized and automated that they'll do everything except fix you coffee while you wait for your results. But for an industry-government group called the Consortium on Automated Analytical Laboratory Systems (CAALS), that's not enough. The CAALS concept, in which entire laboratories will operate without human intervention, controlled from a central personal computer, offers a bold, clear vision of one possible future for computers in science.

Analytical chemistry is approaching a critical time, says Jim Devoe, chief of the inorganic analytical research division at the National Institute of Standards and Technology (NIST), and one of the organizers of CAALS. Industry and government labs are demanding more and more chemical analysis, and the number of qualified chemists isn't keeping up. The only answer, Devoe says, is more automation.

There's plenty of room for it. A case in point is a typical analysis, which might consist of a two-step sample preparation—dissolving the sample in a solution and separating the solution into distinct components—followed by an analysis of the separated solution with a mass spectrometer, for instance, or perhaps optical emission spectroscopy. Although the analysis step is highly automated and reliable, the sample preparation is still often done by a chemist or technician.

Instrument makers are well on the way to automating much of the preparation, too, but that will still leave one big step, Devoe says: putting everything together into a single package. That will entail making systems that can transport the sample from one stage to the next, but that will be the easy part. Harder will be controlling all of the devices from a single computer, so that a scientist can set the system running with one command and not worry about it again until the analysis is through.

At present, each of the automated instruments in a lab is directed by its own software, which is usually incompatible with the software running every other piece of equipment. CAALS is trying to change that. Devoe draws an analogy with the home stereo industry—a consumer picks the components he wants, from whatever maker he chooses, and then can take them home and hook them up together, knowing the combination will work. In CAALS's brave new world of analytical chemistry, a researcher would build his lab out of mix-and-match modules in any combination he pleased.

It's not as easy as it sounds. First there's the problem of convincing instrument manufacturers to settle on a single software standard, when many of them don't even have a single standard inside the company. The consortium includes several major players, including Hewlett Packard, Digital Electronic Corp., Eastman Kodak, and British Petroleum, but they are only a tiny fraction of all the equipment manufacturers. And there are intellectual questions as well: How does one define a "module," for instance? In the stereo world, there are speakers, amplifiers, tape decks and so on, but where to draw the line between different functions in the lab is not so clear.

The rewards of this total automation would far exceed the immediate goal of allowing fewer chemists to do more work. By removing the human factor from sample preparation, it would cut down on mistakes and variability in results. In turn, this would free up the chemists running the lab to vary the settings of the instruments in a methodical way to determine how to get the best measurements. And the standardization would mean that one lab could easily reproduce another lab's setup and check its results.

Devoe compares the automated lab of the future with the well-publicized "smart house" being developed by home builders: Everything will be hooked into a central computer control to make life as easy as possible. In this sense, the "smart lab" epitomizes the real meaning of the computer revolution: It promises to free scientists from much of the daily grind and give them more time for the really hard work: thinking.

—R.P.

Science would like to hear your response to the special section on COMPUTING IN SCIENCE

Name: ______

Title: ______

Institution: ______

Telephone # (optional): ______

Field of scientific specialization: ______

Years in the field: ______

What types of computers do you use in your work?
- ☐ Personal computers
- ☐ Supercomputers
- ☐ Workstations
- ☐ Massively parallel computers
- ☐ Mainframes

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What do you use computers for in your work?
- ☐ Word processing
- ☐ Equation solving
- ☐ Data acquisition
- ☐ Electronic communication
- ☐ Data analysis
- ☐ Access to databases
- ☐ Data visualization
- ☐ Teaching
- ☐ Curve fitting/plotting
- ☐ Other ______

What new hardware or software products would be most useful to you? ______

What subjects and/or products would you suggest including in a future special section on computing in science? ______

Do you think "Computing in Science" should be an annual feature of Science? ☐ Y ☐ N