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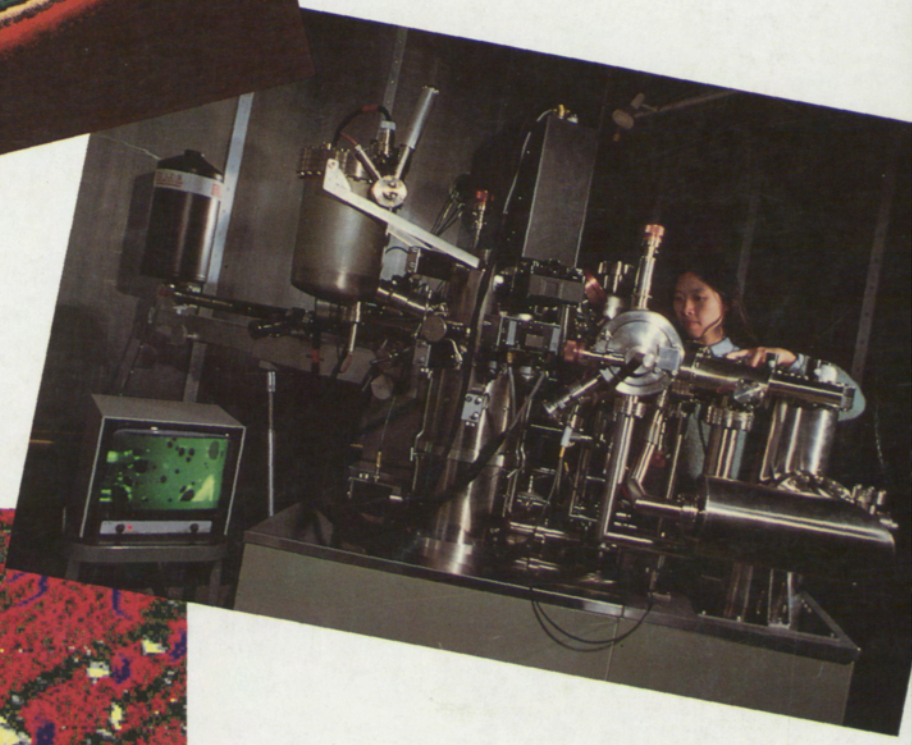
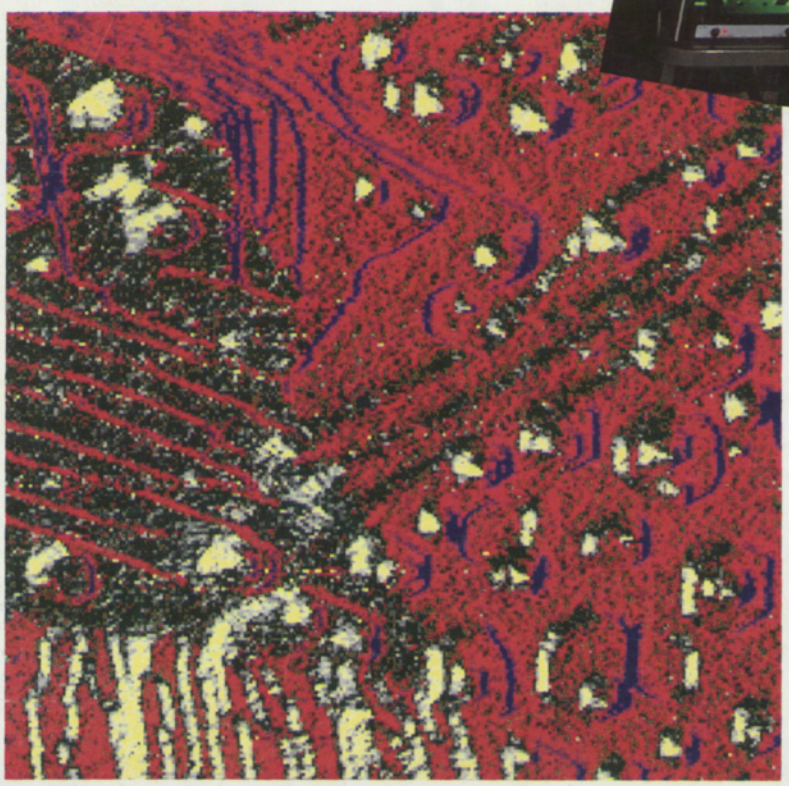




## The Materials Science Center

Cornell's Premier Interdisciplinary Laboratory

# MODULAR PROGRAMS FOR PHYSICAL RESEARCH

by James P. Sethna

*"Available computers can generate amazing movies; the bottleneck is in writing appropriate software."*

Ready-to-use computer software has revolutionized bookkeeping and publishing, but has had much less impact on scientific research.

The available options for graphics—packages to visually display the results of computation—simply do not satisfy the needs of people working at the leading edge of research in the physical sciences. One can find packages to make two-dimensional *x-y* plots, packages for image analysis that will make a Fourier transform from a picture of an orangutan, and ray-tracing packages that are good for drawing teapots. Such software can be used in the presentation of final results, but it has little value as an aid to research. Physicists need visual feedback that is more sophisticated than the bar charts and graphs used in business. They do not need realistic images; cartoons of their results are quite adequate. But they do want to animate their results—adding the extra dimension of time.

A key deficiency of currently available software packages is their lack of flexibility. Research is, by nature, exploratory. When scientists enter unknown territory, unforeseen numerical and graphical problems arise constantly, and researchers must have broad control of their working environment. Also, performance standards are continually advancing, and it is often necessary to tinker with algorithms and graphics hardware.

In addition to being flexible, software should be efficient to work with. Researchers in the physical sciences have spent years individually writing routines in PostScript®, capturing interrupts and mouse input, and controlling the screen on a pixel level. The edit-compile-run-edit cycle that is needed to explore complex simulations and physical phenomena without interactive control is arduous and time-consuming. Software modules with interactive control, which is the hallmark of commercial packages, could greatly facilitate this work. Available computers can generate amazing movies; the bottleneck is in writing appropriate software.

To meet this need, my students and I have been attempting to write a series of modular programs for graphics and numerical analysis that can be used to expedite research in the physical sciences. Our programs are run directly from the Unix shell, and are intended as graphical extensions of Unix. They are written using X-windows, a user interface analogous to Microsoft Windows®, that has become, in the last few years, the official standard of the workstation market. This software development is Cornell's part of an exchange agreement with IBM. Cornell has received, as IBM's contribution to the work, thirty-four RS-6000 workstations with a retail value of over three million dollars, as well as software and staff support.

During the first year of development, our software modules have had a remarkable impact on the research carried out by the theory group in the Laboratory of Atomic and Solid-State Physics. Some have been ported to the Cornell National Supercomputer Facility. Many are now available by anonymous FTP (a File Transfer Program used by Unix) to users elsewhere in the country (see the box on the opposite page).

The examples presented in this article suggest the capabilities of this new software, although the printed page can only suggest the dynamic potential of animated sequences.

### *PlotAtoms:* A Useful Software Package Developed at Cornell

One of the most useful modules is *PlotAtoms*, which was written by graduate student Bruce Roberts. *PlotAtoms* has been of considerable help to researchers studying everything from the structure of quasicrystals to the molecular dynamics of buckminsterfullerene.

The "unit cell" in a quasicrystal is infinite in extent: all attempts to deduce the atomic configurations directly have failed so far. The

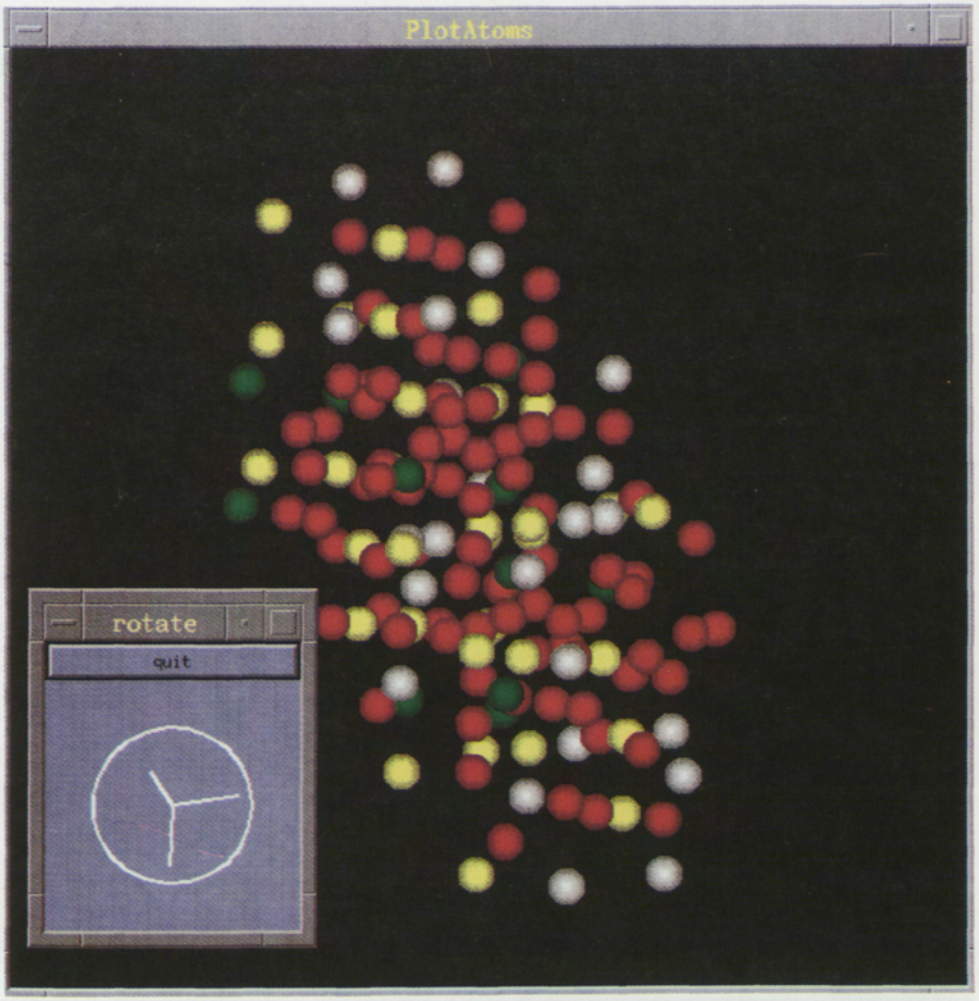



**Figure 1. A unit cell from the crystalline phase of $T_3$(AlMnZn), whose structure is believed to approximate that of decagonal quasicrystals such as $Al_{65}Cu_{20}Co_{15}$ and AlCuNi.**

**Quasicrystals have long-range translational order, but not of the periodically repeating kind found in ordinary crystals. Since the "unit cell" in a quasicrystal is theoretically infinite, direct determination of its atomic configuration is not possible. Instead, researchers extrapolate from analogous crystalline phases with large unit cells, which are rational approximants to the quasicrystal.**

**Here, the red atoms are aluminum, the green atoms are zinc, the white atoms are randomly 80 percent aluminum and 20 percent zinc, and the yellow atoms are randomly 80 percent manganese and 20 percent zinc.**

most successful method for deducing the structure was pioneered by Cornell Professors Christopher Henley and Veit Elser, who worked from analogous crystalline phases with large unit cells. Figure 1 shows a unit cell from one of these crystalline phases, $T_3$(AlMnZn), which is thought to approximate the structure of certain quasicrystals. The three-dimensional atomic coordinates were generated by a general-purpose program written by Sergei Burkov, a visiting professor from the Landau Institute for Theoretical Physics, near Moscow. They were then passed through a series of simple filters, the most interesting of which is *rotate*, an input tool written by graduate student Maynard Handley. Appearing in the lower left side of the screen, *rotate* allows one to select a rotation matrix dynamically, by "rolling" the sphere on which the three unit axes are inscribed. The rotated coordinates are then sorted and passed to

***Readers who have a machine that runs Unix and X-Windows may obtain a copy of the software featured in this article via "anonymous FTP" by using Internet.***

*Type:*

```
ftp ept. msc.cornell.edu
Name: anonymous; Password: (your e-mail address)
cd pub
get LASSPTools.src.tar.Z
get LASSPTools.demos.tar.Z
```

*If you have an RS-6000, you can copy the executables:*

```
get LASSPTools.rs6000.tar.Z
```

*Or if you have a sparc station from Sun you can type:*

```
get LASSPTools.sparc.tar.Z
```

*Then type:*

```
quit
```

*Next, type:*

```
uncompress *
tar –xvf LASSPTools.src.tar. . .
```

*The compressed files are between one and two megabytes each. Uncompressed, the code currently takes 11 megabytes of storage; about half of this consists of examples. The manual pages are in src/manpages.*

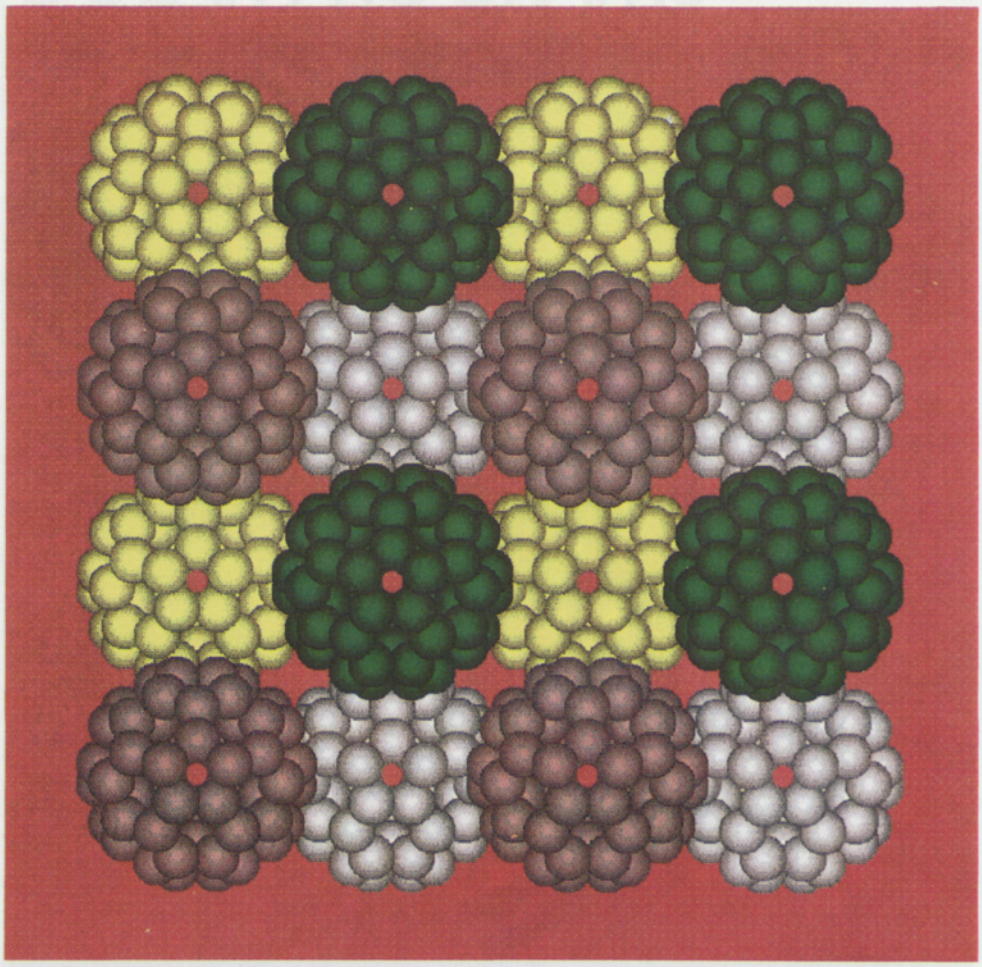


Figure 2. The structure of crystalline buckminsterfullerene. This recently discovered allotropic form of carbon has icosahedral molecules composed of sixty atoms. The substance is named in honor of Buckminster Fuller, inventor of the geodesic dome, which has a similar structure.

Since the molecules are nearly spherical, they continue rotating at temperatures below the point at which the fcc crystal is formed. But at sufficiently low temperature, the slight corrugation of the molecules leads to an ordered state in which molecules in different sublattices assume different orientations. Understanding these phenomena is facilitated by seeing, in real time, how the simulated molecules respond to changes in temperature and pressure at various intermolecular potentials.

This simulation was generated by graduate student Zheng Chen and Assistant Professor Veit Elser.

Developers of modular software for physical research. Around the circle, starting from the left, are graduate student Albert Putnam; undergraduate physics major Jet Ho; graduate students Bruce Roberts and Christopher Myers; James Sethna; graduate student Tom MacFarland; undergraduate physics major David Chin; graduate students J. Ken Burton, Jr. and George Stecher; and undergraduate physics major Eric Lochstet. Visible on the computer screen is *XYInput*, which was developed by Ho.

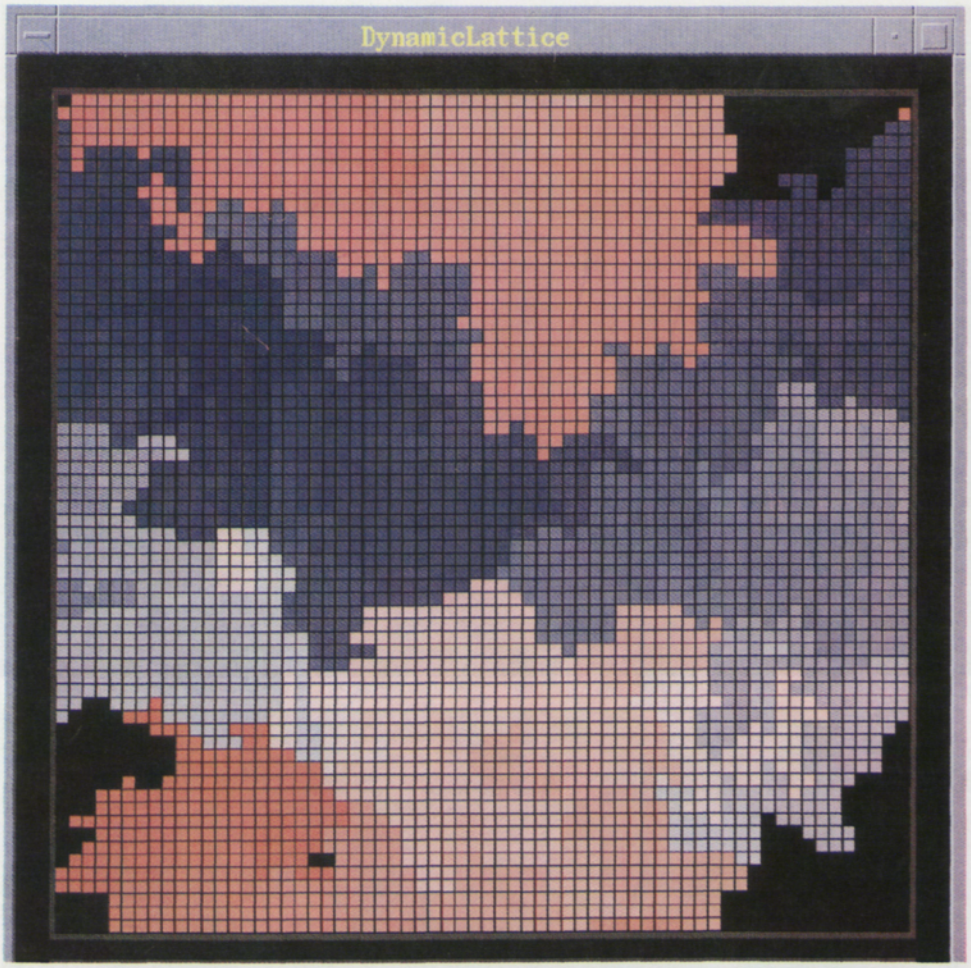



**Figure 3. A snapshot of the evolution of a model charge-density wave as it slides through a period. Many metallic materials, especially those with highly anisotropic electronic structures (quasi-one-dimensional), undergo a phase transition in which electron density and lattice positions modulate spontaneously along one axis. This modulation reduces the net conductivity of the material, sometimes making it into an insulator.**

**At one time the idea was advanced that the modulation, once started, would not stop, and it was proposed as a mechanism for superconductivity. Actually, the opposite is true: the charge-density wave is pinned down by impurities in the material, and does not conduct. However, if a large enough field is applied, the wave can "depin." As the depinning threshold is approached from above, the periodic motion of the wave becomes increasingly jerky—a consequence of large avalanches triggered by the slippage of individual sites.**

**In this simulation, color indicates time of firing: blue sites have already fired, pink sites are currently firing, and red sites have yet to fire.**

**This simulation was generated by graduate student Christopher Myers.**

*PlotAtoms*, which displays them using a series of preformed bitmap images. Turning the unit cell around in all directions makes it possible to glean real information from an otherwise inscrutable mass of atoms.

*PlotAtoms* has also been indispensable in the study of the molecular dynamics of buckminsterfullerene (Figure 2). The software was not just used to make pretty pictures of results, but provided an essential interactive tool right from the debugging stage of the research. *PlotAtoms* has also been used by Professors Albert Sievers and Michael Teter to study molecular dynamics, and by Associate Professor Barbara Cooper's group to study the way ions scatter off surfaces. With the assistance of the Cornell Theory Center, we have used *PlotAtoms* to generate a video tape on ion scattering that graduate student Bruce Roberts showed at the March Meeting of the American Physical Society.

### Software for Studies from Atomic Structure to Earthquake Dynamics

Another very useful module, *DynamicLattice*, was written by graduate student Christopher Myers while doing the research that led to his doctoral dissertation. Later he adapted it for general use. Myers's study of the evolution of charge-density waves (see Figure 3) is one example of what it can do. In addition, its arrow mode makes it useful in studying magnetic spin systems, and its bond mode has been employed in modeling dynamical percolation. Jean Carlson and Jim Langer, faculty members of the University of California at Santa Barbara, have been using it to animate their simulations of earthquake dynamics.

*Grid2Contour*, written by adjunct professor Michael Teter and graduate student Maynard Handley, was used to generate an electron-density contour surface for rutile (Figure 4). The electronic structure was determined us-

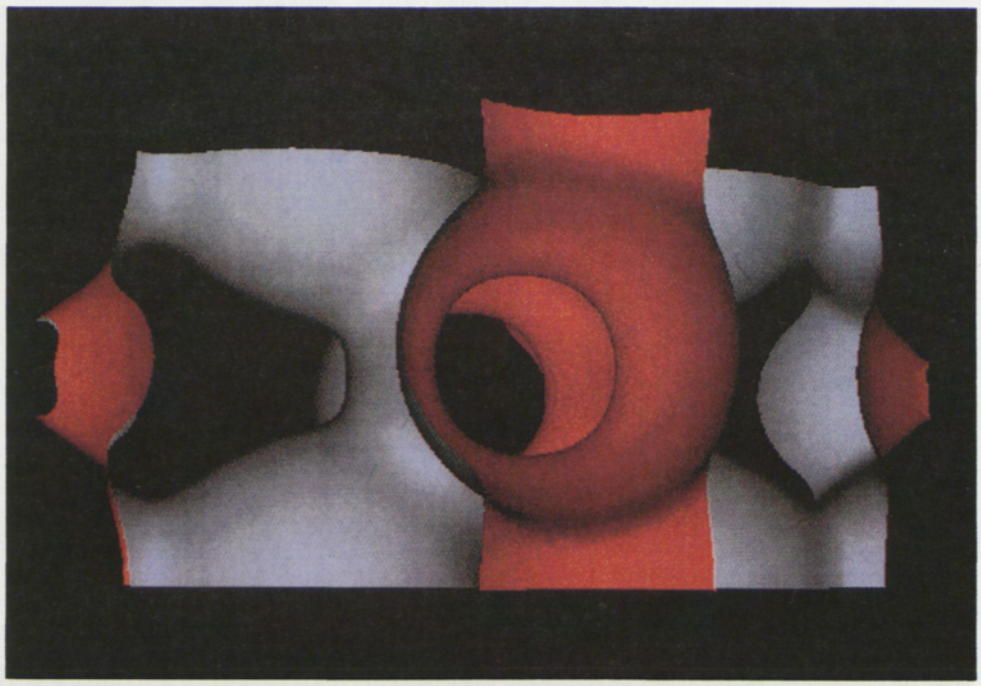


Figure 4. An electron-density contour surface for titanium oxide ($TiO_2$) in the rutile structure. It was constructed with use of *Grid2Contour* from a 3-D grid of electron densities by using an interpolation algorithm and a simple ray-tracing method.

Here the surface chosen for simulation is at the Van der Waals radius of the oxygen atom. The interior of this surface is colored red, and the exterior, blue. The atom shown in the middle is titanium, and the blue tubes represent strongly polarized oxygen atoms.

This simulation was generated by Michael Teter (an adjunct professor) and Douglas Allen, both of Corning Incorporated. Teter likes to compare this calculation with that of stichiovite, a high-pressure form of $SiO_2$ found in meteor craters. Stichiovite shares the rutile structure, but is not as stable. Partly this is because the titanium atom is larger, but mostly it is because the oxygen atoms are not nearly as polarized in stichiovite: the d-orbitals of titanium are important for polarizing the oxygen atoms (the blue tubes) and stabilizing the structure.

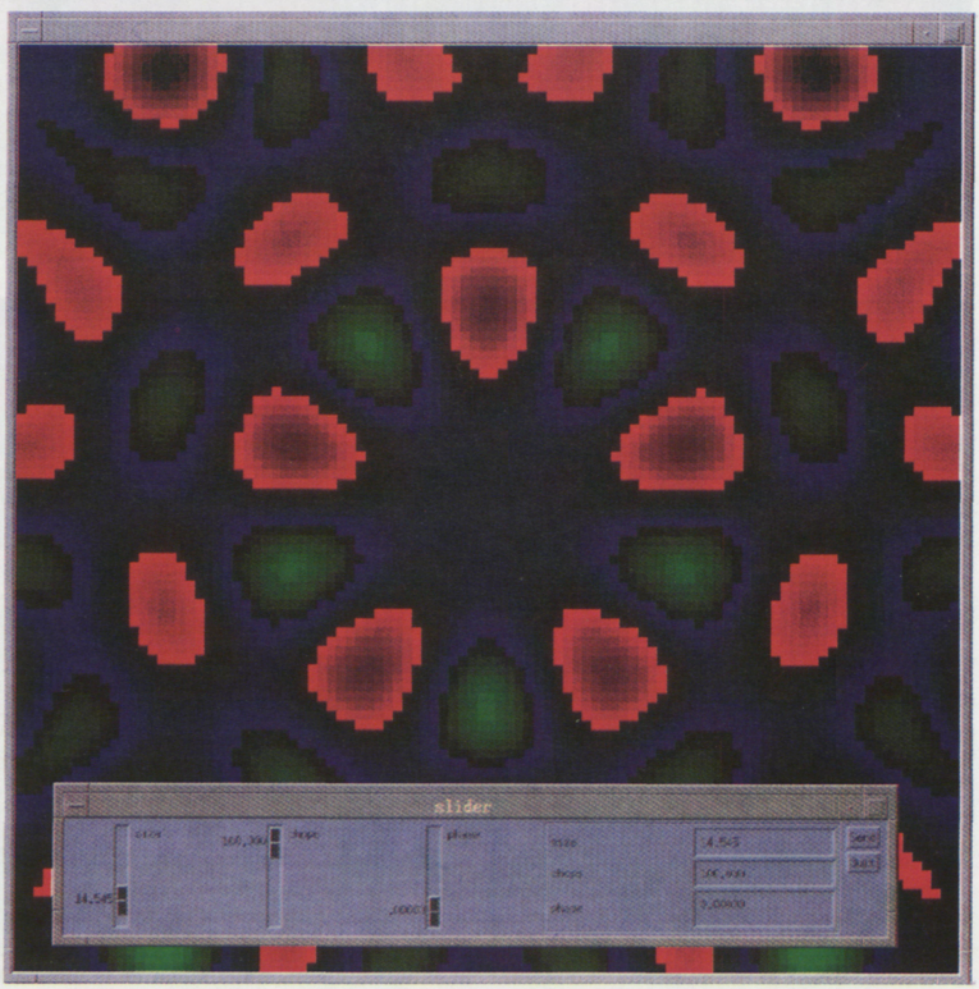



Figure 5. The sum of five cosine waves traveling in the directions defined by the sides of a regular pentagon. The red regions, which may be presumed to represent atoms, are logically and regularly set out, with sensible separations, despite the lack of a periodically repeating pattern.

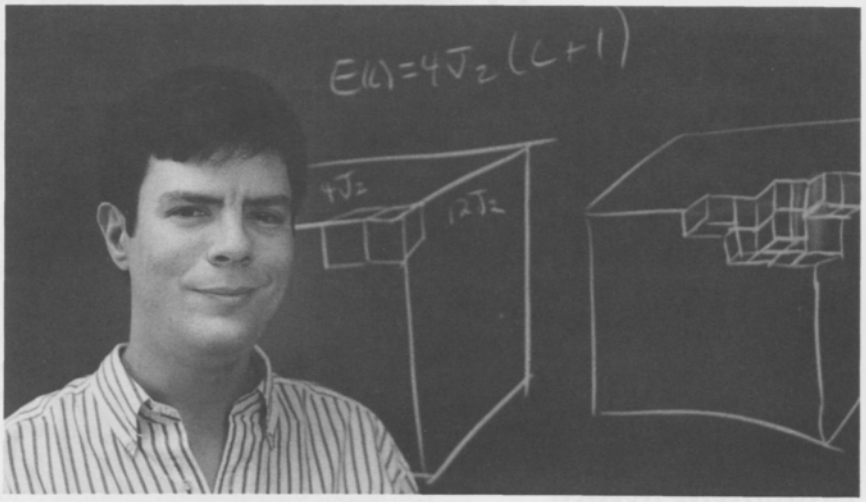
A similar construction was proposed earlier by Professor David Mermin and graduate student Sandra Troian for their theories of quasicrystals.

ing an all-plane-wave local-density code. The contour surface was constructed from a three-dimensional grid of electron densities by using an interpolation method and a simple ray-tracing method that generates a smooth surface without the traditional ambiguities of polygonal surface reconstruction. *Grid2Contour* is about two orders of magnitude faster than traditional ray-tracing methods, but it still takes several seconds to construct a contour surface from a given viewpoint. Frames can be stored up, however, and shown in sequence to form a movie.

Figure 5 shows the sum of five cosine waves in an animated demonstration that can be used in class discussions of quasicrystals. Two important tools are demonstrated: *Slider* and *Matrix2X*. *Slider* was written by undergraduate physics major Jeffrey Osterman and is our most heavily used analog input device. It allows parameters to be adjusted either by sliding on-screen controls with a mouse or by editing numerical values. Three sliders were used to prepare this graphical presentation: the first controlled the size of the quasicrystalline region depicted, the second controlled the resolution (100 x 100), and the third controlled the sum of the phases of the plane waves. The output uses *Matrix2X*, which takes the values of a sequence of two-dimensional grids and displays them as a color animation.

Graduate student Sivan Kartha and I have been using *Matrix2X* to study the "tweed" deformations found in certain metallic alloys. Before undergoing a spontaneous stretching "martensitic" transition, these materials show a cross-hatched pattern in electron micrographs. I showed movies of our model for tweed made with *Matrix2X* in meetings held in the Los Alamos and Brookhaven National Laboratories.

Other important tools developed by our project are *PolyDraw* (written by graduate student Stephen Townsend) and *Poly2ps* (written by graduate student Joel Shore). These packages allow animations of general polygonal constructions to be drawn on the screen or to be output through a laser printer. *PolyDraw* will eventually be used to study polygonalized three-dimensional surfaces, but it already has been invaluable in studying martensites and slow, glassy coarsening in frustrated Ising models. With the aid of the Cornell Theory




Center, Joel Shore developed a videotape showing this coarsening, and I presented it recently during talks delivered at the University of California. Much physical research has been done with the aid of transparencies, but animations are the transparencies of the future.

Numerical analysis tools currently under development are filters for interpolation and smoothing, filters for nonlinear fits to data (using *Slider* to interactively find approximate fits, and nonlinear least-squares to fine-tune), and filters for matrix manipulations, Fourier transforms, and eigensystems.

In a grand view, we hope to do for numerical analysis and graphics what most operating systems do for file manipulation and text processing. We hope to provide the obvious components necessary for use in a wide variety of scientific and engineering applications. ■

*"... we hope to do for numerical analysis and graphics what most operating systems do for file manipulation and text processing."*

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*James P. Sethna, an associate professor of physics, has been at Cornell since 1984. A member of the Laboratory of Atomic and Solid State Physics as well as the Materials Science Center, he conducts research in the areas of glasses, defects in liquid crystals, quantum tunneling, and dynamical systems and has published some fifty papers.*

*Sethna received the B.A. degree in physics from Harvard University in 1977 and the Ph.D. from Princeton University in 1981. Before joining the Cornell faculty, he did postdoctoral work here and at the Institute for Theoretical Physics at Santa Barbara.*

*In 1985 he received a Sloan Resesarch Fellowship and a Presidential Young Investigator Award, which provided research support for five years through the National Science Foundation.*