

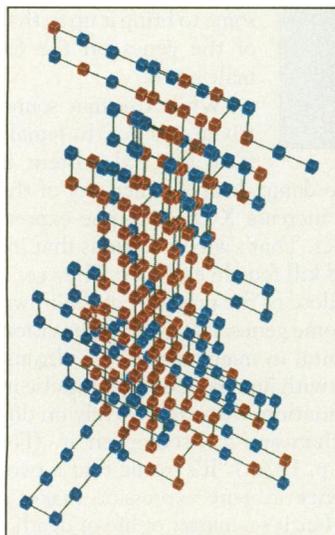
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protease, which is the target of promising state-of-the-art drugs. "As your model gets better and more HIV-1-like and the number of agents increase, people will use the models more," Sodroski predicts.

Primate AIDS researchers are impressed by the work. "I think it's wonderful," says Michael Murphey-Corb of the Tulane Regional Primate Research Center. "We really do need this." Murray Gardner of the California Regional Primate Research Center says this is the first documented evidence that SHIVs can produce disease. RT-SHIV may "open the door" to using monkeys to test new AIDS drugs, especially in combination, he says. "Now everything just goes into humans willy-nilly."

### Folding Proteins Fast

"The single problem [in biology] with the very largest payoff at this point," says George Rose, a biophysical chemist at Johns Hopkins University, "is a practical way to predict protein structure from amino acid sequence." Now a team from Sandia Na-



**Fast fold.** Computer model for protein triphosphatase isomerase, determined from its amino acid sequence in less than a second. Red and blue boxes are water-hating and -loving amino acids.

tional Laboratories in New Mexico has an algorithm that may come close to hitting pay dirt.

Proteins can be composed of sequences of hundreds of amino acids, yet protein function seems to be determined in large part by how those sequences fold up into biologically active conformations. And the number of ways a string of amino acids can be folded is "astronomical," says molecular biologist Jonathan King of the Massachusetts Institute of Technology.

Therefore, several groups are working on algorithms that for the first time will make it possible to predict protein structure—and do it fast—using a computer. Rose, who published the first such algorithm last winter, and Ken Dill, head of the Center for Statistical Physics of Macromolecules at the University of California, San Francisco, have both been working on algorithms that have reduced the time it takes to sort out the structure of small proteins to days or weeks.

But perhaps the most intriguing algorithm comes from mathematicians Sorin Istrail and William Hart at Sandia, who have combined their mathematics with Dill's biological model of protein folding to create an algorithm that may turn out to be several orders of magnitude faster than the competition. The algorithm goes about finding a protein's ultimate shape by finding

## Materials Science—Live on the Net

Why isn't there more good course software available on the Internet? Materials scientist John Russ and his students at North Carolina State University know one reason: Putting it on-line takes a huge amount of work. It's taken Russ 5 years, with student help, to develop an electronic version of an entire first-year undergraduate materials science course.

The course, "Visualizations in Materials Science (VIMS II)" makes for a giant Web site: <http://vims.ncsu.edu>. Each of the 20 on-line chapters has interactive exercises and illustrative materials, including videos, animated simulations, graphs, diagrams, cartoons, and photos. In the chapter on "nucleation and growth," for example, one can watch a microscope's view of ice dendrites forming in water. The chapter on "ferrous alloys" has a 23-part video tour of the NuCor steel plant in Darlington, South Carolina, complete with sound for those with the right software. "In the science area I'm not aware of anything this complete on the Internet,"



says Russ. In the past few weeks, he says, "we've had people coming in from literally all over the world using it—[there have been] about 12,000 hits a week on it."

Russ began the project in 1990, developing computer graphics and animations to supplement his teaching. With funding from the National Science Foundation, he turned these graphics into a CD-ROM to accompany the course. Last month, concerned that many people don't have access to CD-ROM players, Russ put the course on the Internet.

"People like John Russ are really ahead of the pack," says engineer Mark DeGuire of Case Western Reserve University. James Wittig, associate professor of materials science at Vanderbilt University, who has used the CD-ROM with his students, notes that most professors simply do not have the time or the resources to do what Russ did. More such courses will require collaboration by "faculty with similar interests from different universities," he says.

the minimum energy state of the molecule. It does that by doing what proteins do: first making a big fold in the amino acid chain, which is equivalent to the protein collapsing on itself. It then assumes that hydrophobic amino acids, which dislike water, will migrate toward the center of this fold. There they will join with other hydrophobic amino acids. This stabilizes the protein.

The Sandia algorithm, says Dill, has not yet been validated by testing on proteins with known conformation. But he calls it "a very nice step forward in the computerology of proteins."

### Shrinking National Labs

As Congress continues to hammer out a thinner budget for the Department of Energy for fiscal year 1996, most of the nine major DOE labs have reported recent or imminent layoffs. The labs are moving to show they can reform themselves as members of the House Science Committee contemplate measures such as consolidating labs or limiting the kinds of research they do (*Science*, 15 September, p. 1510).

The latest big hit came on 13 September at Los Alamos National Laboratory, when it announced the layoff of 781 employees. About 83% of the jobs cut were support positions; the rest were scientific or technical. The objective, says Los Alamos

spokesperson James Danneskiold, is to increase productivity in relation to expenditures by raising the ratio of scientists and technicians to administrative and support staff.

Personnel layoffs and attrition to date:

- Pacific Northwest National Laboratory—About 900 positions, mostly support staff, were eliminated earlier this year.

- Brookhaven National Laboratory—90 employees throughout the lab will be laid off before November.

- Idaho National Laboratory—1250 positions were eliminated a year ago; no further layoffs are planned.

- Sandia National Laboratory—plans to lose about 600 positions from retirement and normal attrition between now and October 1997.

- Argonne National Laboratory—195 positions eliminated last year, 102 through early retirement.

- Lawrence Berkeley National Laboratory—150 support positions were cut in August, and about 13 additional layoffs were announced on 20 September.

- Lawrence Livermore National Laboratory—Staff has been reduced by 15% in the past few years.

- Oak Ridge National Laboratory—22 layoffs this summer from research and support positions.