

Turtle recovery could take many decades

Under current protective laws, it would take at least 70 years to achieve a 10-fold increase in populations of the loggerhead sea turtle off the coast of the southeastern United States, according to a new computer forecast. Wider use of turtle excluder devices (TEDs) — trapdoor-like mechanisms that allow sea turtles to escape shrimp-trawling nets — would reduce this recovery time by only 30 to 40 years, the forecast indicates.

Biologists consider a 10-fold population increase crucial to saving this threatened species.

The new computer model is the first to take into account the differing effects of TEDs on the survival of loggerhead turtles of various ages and sizes, says Selina Heppell, a biologist at North Carolina State University in Raleigh. Heppell described the model last week at the joint annual meeting of the American Institute of Biological Sciences and the Ecological Society of America, held in Honolulu.

Because TEDs are less effective in saving smaller, younger turtles, she says, the model suggests that fewer than anticipated numbers of loggerheads will survive to reproductive age.

Most TEDs consist of a panel of metal bars inserted into a trawling net at an angle leading up to a hole in the top of the net. The bars are designed to allow shrimp to pass through and accumulate in the sack-like end of the net, while diverting larger marine animals — such as sea turtles — up and out of the net through the hole.

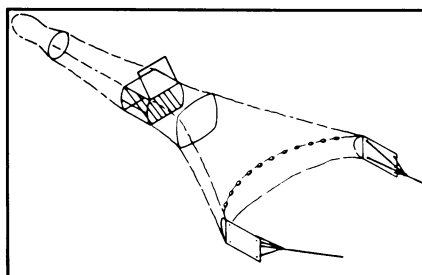
The U.S. National Marine Fisheries Service (NMFS) estimates that TEDs have slashed by 67 percent the annual mortality rate of sea turtles caught in trawling nets in U.S. coastal waters since the 1988 enactment of a federal law requiring shrimp trawlers to use the devices during selected times of the year in most offshore areas. Despite the use of TEDs, however, the NMFS projects that at least 4,360 sea turtles inhabiting U.S. coastal waters will drown in trawling nets this year.

Heppell's forecast rests on the assumption that TEDs reduce the mortality rate of net-trapped juvenile loggerheads by only 34 percent each year, because these smaller turtles sometimes get swept between the bars of the devices and become caught in the nets. This potentially fatal generation gap skews the demographics of the loggerhead population toward older turtles with fewer remaining reproductive years, Heppell says. This, in turn, slows the recovery rate of the species as a whole, she asserts.

"TEDs have had a very positive effect

on increasing the population [of loggerhead turtles]," Heppell says, "but 70 years is a longer time to see a 10-fold population recovery than we'd expected." She adds that although the number of nesting loggerheads has increased within the past three years, indicating the overall benefits of TEDs, "we have to be a little cautious in saying we've found the answer to saving the [loggerhead] turtle population. . . . It's going to take a long time."

Last April, the NMFS proposed new regulations that would expand the requirements for TED use by mandating trawlers to use TEDs year-round at all U.S. inshore and offshore locations. This would achieve a 97 percent reduction in



A turtle excluder device (slanted bars) provides an escape hatch for sea turtles accidentally swept into a shrimp-trawling net.



A loggerhead sea turtle on the beach.

trawler-related turtle mortality, according to agency estimates.

However, the proposal does not call for new TED designs less likely to trap juvenile loggerheads. Nor does it address what Heppell describes as a potential threat to all sea turtles: the harvesting of sargassum, a type of seaweed that grows in floating mats.

Commercial harvesting of these vast mats for use in pharmaceuticals or livestock feed could destroy an important habitat for "small juvenile" sea turtles, Heppell says. According to her model, this category of juveniles constitutes the second most important age group for the recovery of the loggerhead population. Increasing the mortality rate of small juveniles through sargassum harvesting could delay a 10-fold increase in loggerheads to 140 years, Heppell projects.

— C. Ezzell

Shaking and baking to atomic positions

An expert crystallographer can take literally years to work out, largely by trial and error, the positions of atoms in a given molecule. An innovative, computer-intensive method of extracting information directly from X-ray diffraction data now offers the possibility of cutting that time to hours.

In a recent test of this new method, researchers needed only a few hours of computer time to provide the information needed to find the positions of 104 atoms in pairs of molecules of a compound related to the immune-suppressing drug cyclosporin. Using more conventional methods, Russian scientists had spent nearly a decade trying to determine its structure — without any success.

The researchers who developed the technique, led by Herbert A. Hauptman of the Medical Foundation of Buffalo and the State University of New York at Buffalo, announced their achievement at last week's American Crystallographic Association meeting, held in Pittsburgh. This success marked the first time the researchers had applied their technique to a large molecule with a previously unknown structure.

The technique has the potential to dramatically accelerate the designing of drugs for specific purposes, a process that relies on knowledge of chemical structures of molecules, Hauptman says.

In X-ray crystallography, researchers bombard a single crystal of a given substance with X-rays of a certain wavelength. The orderly rows of atoms within the crystal deflect these X-rays in particular directions to produce a distinctive pattern of spots on a photographic plate.

The positions and intensities of these spots, which could number in the thousands, provide information about the locations of atoms within molecules of the given substance. But that isn't enough to draw a complete three-dimensional portrait of the unknown molecule. Because they don't know the times when X-rays arrived at each spot, crystallographers generally lack information about the so-called phase relationships of the diffracted X-rays. And because they need both intensity and phase data to find a molecular structure, experts must often rely on informed intuition to aid in unraveling a molecule's structure.

Several years ago, Hauptman proposed a mathematical formula that he claimed could be used for zeroing in on the missing phase information. This complicated formula exploits subtle relationships between phases and measured diffraction intensities. If one could minimize the value of this complicated expression containing thousands of variables, one could solve the phase problem.

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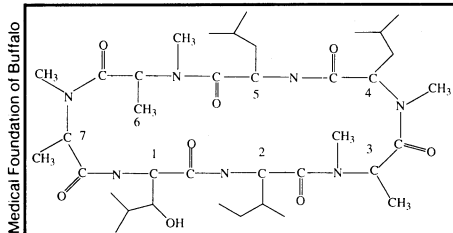
Heppell

To make the scheme workable, computer scientist Russ Miller of SUNY-Buffalo and his co-workers developed algorithms specially designed to run efficiently on computers consisting of large numbers of parallel processors, which operate simultaneously while working on different pieces of a problem.

The result was a "shake-and-bake" strategy, which starts with "trial" molecules consisting of random arrangements of atoms, subject only to chemical constraints. "You essentially toss the atoms in a shoebox with enough chemical knowledge to make sure the arrangement makes chemical sense," Miller says.

The computer calculates the phases associated with these atomic positions. Then it randomly perturbs the resulting phases in such a way as to provide a slightly lower value for Hauptman's formula, and computes the new positions of the atoms. The atoms, in turn, move slightly, leading to another calculation of the phases, and so on. The computer may go through as many as 200 such phase-position cycles for each initial arrangement of atoms.

In April, the researchers used this technique to solve the structure of the antibiotic gramicidin-A, which contains 317 atoms, excluding hydrogen. They accomplished in a matter of weeks what had originally taken David Langs, a senior research scientist at the Medical Founda-



tion of Buffalo, 10 years to work out using other methods.

Last month, having a few days of free time between projects, Miller came to Langs asking for crystallographic data on which to test his newly refined version of the structure-determination algorithm. Langs, highly skeptical that anything would come of it, suggested finding the structure of a molecule that had long stymied Russian scientists. Over two years, Langs himself had tried half a million possibilities with no success.

"I put the data into the program before I went to bed at night, and the next morning I looked through the results," Miller says. One of the 64 random arrangements of atoms with which he had started gave a value for Hauptman's formula that was significantly lower than the others, indicating the right answer.

This particular trial result provided sufficient information for Langs to work out the details of the molecule's structure in only a few hours (see diagram). Out of

Positions of 52 atoms (excluding hydrogen) in one of a pair of molecules having the same formula but two different conformations in a crystal.

the millions of possible atomic arrangements, Miller's algorithm had converged on the correct structure with remarkable efficiency. It was like looking for a needle in a haystack with the advantage of having a magnet on hand.

Subsequent tests involving 640 random atomic arrangements produced two additional results that converged to the same, correct molecular structure. "I had been lucky," Miller says. "The first one happened to come out in the first batch of 64." Each set of 64 trials took about 1.5 hours on a multiprocessor computer known as the CM-5 Connection Machine.

After this initial success, Langs provided Miller with a second unknown structure related to the first but deemed more difficult to solve. "We gave it a shot, and the answer emerged just as rapidly," Miller says.

"It was quite remarkable to us. It made believers out of a lot of people," says Jane Griffin, head of molecular biophysics at the Medical Foundation of Buffalo. "But we still have a lot of research to do in extending [the method], seeing how high the resolution of the data has to be, and solving a variety of other problems."

— I. Peterson

Laser process shapes microscopic parts

By combining advances in lasers, chemistry, and computer-aided design and manufacturing techniques, scientists have scaled machining down to microscopic proportions.

This new technology makes possible machined pieces one or two orders of magnitude tinier than the finest parts crafted by watchmakers, says Daniel J. Ehrlich, a physicist at the MIT Lincoln Laboratory in Lexington, Mass. Ehrlich and Theodore M. Bloomstein, a graduate student in electrical engineering at MIT, describe their three-dimensional micromachining process in the Aug. 10 *APPLIED PHYSICS LETTERS*.

Using this process, "you can do almost anything and make any shape both along the [surface] and the depth," comments Howard R. Schlossberg, a physicist with the Air Force Office of Scientific Research in Washington, D.C.

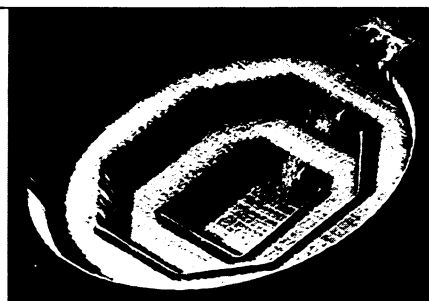
To make their three-dimensional designs, Ehrlich and Bloomstein rely on a computer to guide a laser as it scans a piece of silicon. First they use computer-aided design and manufacturing (CAD/CAM) software to draw and scale a part. A second program slices that computer blueprint into many parallel planes. The computer notes the coordinates of the part in a given plane and then directs

the laser to etch plane by plane, leaving silicon only at those coordinates.

For shaping, Ehrlich and Bloomstein place a newly cleaned silicon crystal into a vacuum chamber and blow chlorine through the chamber. The instant the laser hits the silicon surface, it heats that spot to about silicon's melting point. The heated silicon combines with chlorine atoms hitting it and escapes as a silicon chloride gas. "Among reactions that occur on a surface, it's among the very fastest," Ehrlich says. The researchers then pump out this gas.

The computer can direct the laser to any 1-micron location on a square surface 256 microns wide. The laser then etches down in 1-micron steps. It can hit up to 20,000 spots per second and moves at a rate of 20 millimeters per second. The longer the laser dwells at a spot, the more deeply it etches the silicon, enabling the researchers to shape the part in the third dimension. Higher pressures of chlorine also speed etching, Ehrlich says. In addition, varying the chlorine pressure lets the researchers control the part's final texture.

The MIT group got the idea for this process in part from recent advances in stereolithography, in which a computer-directed laser causes liquid plastic to



Laser-induced chemistry first shaped the micron dimensions of this multilevel silicon "hot tub," then deposited a pattern of metal (white) inside it.

solidify into a particular shape. "We also have begun to build [up] three-dimensional things," says Ehrlich. For example, they have used the laser and a technique called chemical vapor deposition to lay down patterns of platinum or cobalt in the newly shaped silicon.

Ehrlich expects manufacturers to use the micromachining technique to make microscopic prototype parts, molds, and stamping tools. The MIT researchers have produced plastic parts from these micromolds, and they hope to use those parts to make valves and pumps for implantable medical devices. They are also refining the technique for micromachining metals and ceramics.

— E. Pennisi