The Columbus Dispatch

Mimicking mollusks

With help of supercomputer, researcher hopes to unravel how nature forms shells, teeth and bone

Sunday, January 30, 2011 02:57 AM

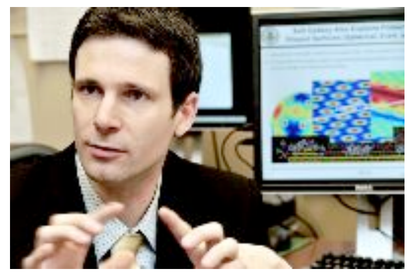
BY SPENCER HUNT

THE COLUMBUS DISPATCH

When most of us pick up seashells on the beach, we don't think much about the process in which they formed or what that means in the greater scheme of things.

Then again, most of us are not polymer engineers.

Hendrik Heinz is, and when he looks at a seashell, he sees a genetic puzzle that if unlocked could help repair broken bones, replace lost teeth and even create longer-lasting fuel cells.



UNIVERSITY OF AKRON

Hendrik Heinz, polymer engineer

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Florida tree snail shells

Growing shells for protection from harsh environments and predators is an evolutionary trick mussels mastered millions of years ago. Humans and animals use a similar process to grow and maintain their teeth and bones.

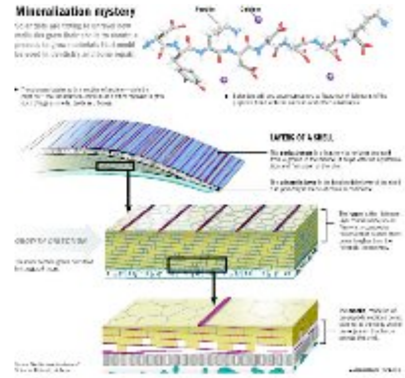
But knowing that this process works is a far cry from understanding it.

Or replicating it in a lab, for that matter.

But that's exactly what Heinz is trying to do. So he went to the Ohio Supercomputer Center in Columbus, where a cluster of computer processors can perform as many as 75 trillion calculations per second.

Over the next five years, the supercomputer will run simulations focused on proteins - complex organic molecules expressed by DNA - that bond to microscopic particles of calcium and metals.

In animals and humans, these proteins bond with minerals and help



organize the particles into tough specific structures, such as an incisor, a femur or a ridged shell.

"The hardest thing is to look at how these components are arranged," said Heinz, a professor at the University of Akron. "It all goes together in a very organized state and there are many contributions to that."

It's a puzzle in which scientists have all the pieces, but don't know how to fit them together.

One peptide, a segment of a protein molecule, contains as many as 20 different amino acids, each of which could bond in as many as 20 different ways to a particle of calcium or some other element.

"That's 20 {+2}{+0} possibilities," Heinz said. "That's a huge number."

The process also occurs in a matrix that involves thousands of similar peptides in an environment affected by water and temperature.

Efforts to recreate the process in the lab involve randomly selecting protein combinations and mixing them with minerals to see how they react, said Mehmet Sarikaya, director of the University of Washington's Genetically Engineered Materials Science & Engineering Center.

"For us, it's mostly trial and error. We know which (peptides) are good, but we don't know why they are good," Sarikaya said. "The key is controlling the protein sequence so we can control the microstructure of the mineral."

That's where the supercomputer comes in.

Its brain can run simulations to see how successfully different amino acids could bond with different particles. The supercomputer's hyper-processing power is needed to run all the variables quickly, said Ashok Krishnamurthy, the supercomputer center's interim co-executive director.

"To get more realistic answers, you need to include more and more molecules in the simulation," Krishnamurthy said. "The more molecules there are, the more and more complicated the equation."

Sarikaya said he hopes Heinz's research could offer a more specific set of peptides to test in the lab.

"There are no clear-cut guidelines scientists can follow to design protein-protein interactions," Sarikaya said. "This could save a lot of time. This could give us guidelines."

Heinz, who has conducted related research at the supercomputer center since 2007, received a two-year, $430,000 National Science Foundation grant last summer to further study how organic molecules can help build "inorganic components."

An outline of the molecular mechanics used to build things such as shells or bones, Heinz said, could lead to new techniques to create better, longer-lasting dental prosthetics or ceramics.

It also could lead to new treatments to help speed the repair of broken bones.

Another more far-flung possibility could involve attaching organic enzymes to the metal electrodes in fuel cells in an effort to help them last longer and transfer energy to motors from biofuels in the cells.

Sarikaya said the medical possibilities are incredible.

"If you could figure this out, osteoporosis wouldn't be a problem," he said. "Tooth decay wouldn't be a problem."

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