RLE currents

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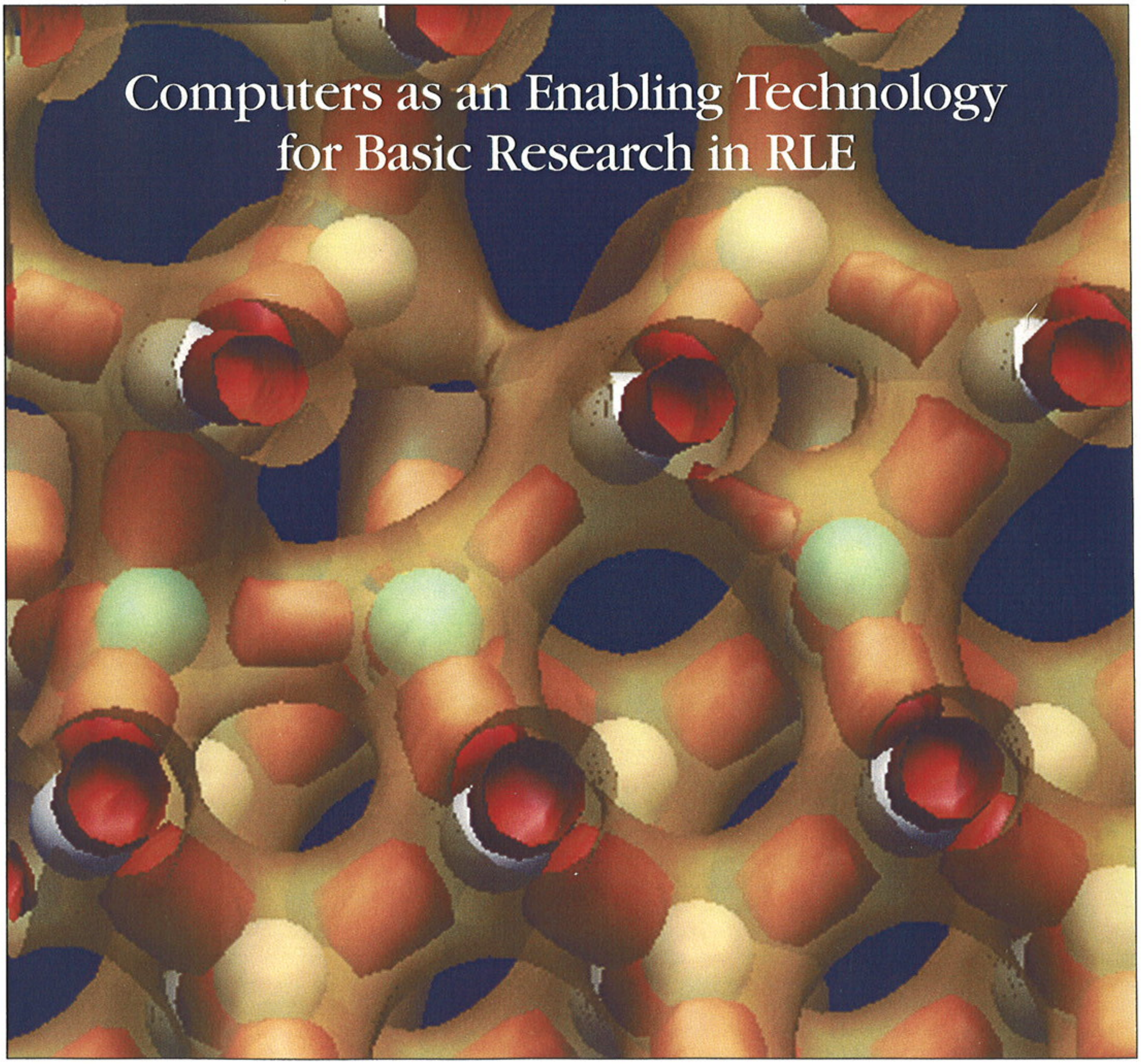
The Research Laboratory of Electronics at the Massachusetts Institute of Technology

Computers as an Enabling Technology for Basic Research in RLE



Director's Message

We all realize that computers form an increasingly large part of the set of tools we use to do our work. In this issue of ***currents,*** we illustrate not only the incredibly broad scope of this impact on RLE's research, but also the way in which the nature of certain research topics leads to new computational resources, both hardware and software. In this way, computing has become a vital part of our research enterprise, and we are creative exploiters of it at all levels, from the smallest low-power circuits to the largest highly parallel multiprocessor machines. Not only do we find computing central to the modeling, simulation, and visualization of inanimate physical systems, we also increasingly find it at the heart of our work on biological systems, including human-computer interactions. In addition, while experimentally derived data often drives modeling and simulation, innovative "computer experiments" also suggest new areas of exploration for physical effects predicted by fundamental theory.

Given these rapidly evolving techniques, it is not surprising that the constant interplay of research and teaching in RLE has led to new environments for learning. These new learning environments facilitate direct interaction between students and the simulated behavior of entities under study, be they electronic circuits or biological cells, so that students can build their own internal models in a highly personal way. From all these examples, we see that computing is an integral part of our research enterprise, providing an important component in how we seek to understand and learn the nature of our world.

Jonathan Allen, Director, Research Laboratory of Electronics

Throughout history, scientists have searched for the fundamental laws that govern our universe. In their search, four different scientific methods have been used to carry out research in the quest for answers. The first is called *observational science,* where a situation or phenomenon is studied and then carefully documented. Observational methods are used in many natural sciences, for example, in animal behavior studies, astronomy, and the geological sciences. In the second method, *experimental science,* experiments are carried out to provide insight into basic scientific principles. Here, it is important to use control groups for comparison and to keep as many factors as constant as possible to isolate cause and effect. Examples of experimental methods include tests to determine the appropriate chemical concentrations for new medicines or the comparative testing of airplane design in a wind tunnel. The third method involves *theoretical science,* where a theory or law is hypothesized and then proven by additional research or mathematics. The complex equations that describe certain properties or phenomena in the physical sciences, such as the familiar $e=mc^2$ formula of Einstein's theory of relativity, are examples of theoretical science.

Until recently, these three methods were the only ones typically used for most scientific investigations. The fourth

Front cover illustration: *The core of a dislocation in crystalline silicon as seen from the perspective of its electrons. Calculated by physics graduate student Gabor Csanyi with the special density-functional language DFT++ developed in Professor Tomás A. Arias' group, the image contains reddish-gold regions corresponding to atomic bonds and spheres that represent the cores of the silicon atoms. Greenish atoms are at the center of the dislocation. The surprising result of this image is seen in the white atom located slightly above and to the right of center. This atom, which has two greenish atom neighbors, has a very subtle structure rarely found in crystalline silicon. With five neighbors and five bonds, it is known as a "floating bond" and previously had only been theorized to exist in amorphous silicon. Calculations for this research ran on the experimental Xolas shared memory processor at MIT's Laboratory for Computer Science, which took several weeks to produce the results shown above.*

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