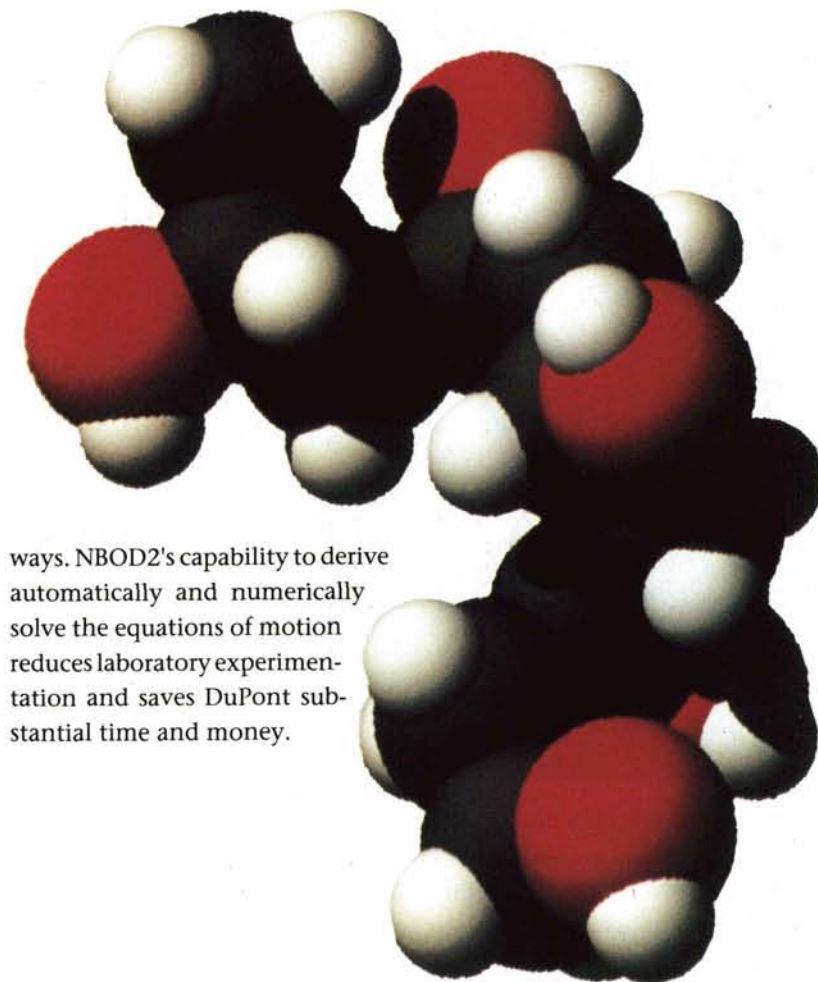# Drug Research

Analysis of the dynamic characteristics of a complex system — a spacecraft, for example — is usually best accomplished by study of a simulation model with the aid of a specially developed computer program. An example is a program developed by Goddard Space Flight Center to solve equations of motion for coupled N-body systems.

Drugs are complex systems, too, and at E.I. DuPont de Nemours & Company, Wilmington, Delaware, researchers are using the Goddard program to model the energy and motion of drug/enzyme bonding as part of the process of designing new drugs. The program was supplied to DuPont by NASA's Computer Software Management and Information Center (COSMIC)®. Located at the University of Georgia, COSMIC routinely makes available to industrial and other clients computer programs that have secondary availability.

Drugs affect biological systems — such as the human body — by interacting with enzymes, complex proteins that catalyze specific biochemical reactions at body temperature. A drug "fits" into an enzyme's receptor slot like a key into a lock and dictates new behavior to the enzyme, thereby affecting the biochemical process that the enzyme catalyzes.

The shape of a drug molecule determines the coupling between the drug and a particular enzyme. Once attached, the drug may change shape and slot into new bonding situations with the enzyme. Each bonding stage has specific biochemical results.

At DuPont, researchers model potential drugs as a series of aggregates (elements) and springs (bonds), as in the accompanying photo. The NBOD2 program then analyzes the vibrational and static motions of these independent components. The information supplied by NBOD2 is used to design specific drugs to interact with particular enzymes in designated

ways. NBOD2's capability to derive automatically and numerically solve the equations of motion reduces laboratory experimentation and saves DuPont substantial time and money.

® COSMIC is a registered trademark of the National Aeronautics and Space Administration.