Cornell Theory Center's Biomedical Resource is renewed

FOR RELEASE: Jan. 28, 1997

Contact: Linda Callahan
Office: (607) 254-8610
E-Mail: cal@tc.cornell.edu

ITHACA, N.Y. -- A five-year, $5 million grant for the Parallel Processing Resource for Biomedical Scientists at the Cornell Theory Center has been renewed.

The Parallel Resource, funded by the National Center for Research Resources (NCRR) at the National Institutes of Health, is an interdisciplinary, multi-institutional collaboration aimed at applying high-performance computing and communications to support advances in biomedical applications.

In addition to Malvin H. Kalos, Theory Center director, co-principal investigators of the Parallel Resource include Thomas F. Coleman, professor of computer science, and Harold A. Scheraga, the Todd Professor of Chemistry Emeritus, both at Cornell.

During the last five years, the Parallel Resource has contributed to several breakthroughs in biomedicine. Jon Clardy, Cornell professor of chemistry, and his collaborators announced in July that they had determined the structure of a complex of two proteins -- FRAP and FKBP11 -- bound to a small molecule called rapamycin. The existence of this complex has important implications in the design of better immunosuppresive drugs. Clardy's group has taken advantage of the Parallel Resource's graphics and animation expertise. Images created by visualization specialist Richard Gillilan have appeared in the journal Science and other publications.

A second major discovery involved the development of non-linear laser microscopy, a new type of microscopy that shows the activity and behavior of living cells under a variety of conditions. Staff at the Developmental Resource for Biophysical Imaging and Opto-Electronics, another Cornell-based NCRR-funded program run by Watt W. Webb, professor of applied and engineering physics, uses graphics technology developed in part at the Theory Center to reconstruct and analyze optical sections collected by the imaging technique.

"The Parallel Resource provides the biomedical community with extraordinary parallel computing capabilities," Kalos said. "Equally important to our research community is the expertise of our technical staff, who are helping scientists open new horizons of discovery through virtual reality tools."

Biomedical scientists have tackled a number of projects with the support of the Parallel Resource, including:

-- simulations of the distribution of radiation doses in cancer patients;

-- modeling cardiac arrhythmia;

-- developing new techniques for molecular-level details regarding reactions in solution and in enzyme active sites;

-- studying new methods in quantum chemistry;

-- understanding how electronic properties influence the reactions of chemical mutagens and carcinogens with DNA.

In a number of instances, the biomedical applications are driving development of virtual reality capabilities in the Theory Center's Visual Insight Zone (VIZ). The VIZ is currently being used to explore molecular docking technology for use in the design of drugs to treat Chagas Disease, a debilitating illness affecting more than 18 million people.

Kalos said that the next five years will see a broadening of the Parallel Resource's reach into more fields of biomedical research. For example, a collaborative project with Robert Waag at the University of Rochester is aimed at developing techniques for the reconstruction of high-resolution, quantitative images that improve as well as extend the utility of ultrasound as a diagnostic tool in medicine.

"This research, which combines expertise in computational optimization, inverse problems and instrumentation, is a rare opportunity for a breakthrough in ultrasonic imaging," Kalos said.

In another new Parallel Resource project, Nobel laureate Herbert A. Hauptman, of the Hauptman-Woodward Medical Research Institute and the State University of New York at Buffalo, will continue development of his "Shake-and-Bake" algorithm for crystal structure determination. Hauptman, who received the Nobel Prize in Chemistry in 1985, is collaborating with principal investigator Scheraga and with researchers at Cornell's MacCHESS facility, which applies the Cornell High Energy Synchroton (CHESS) to macromolecular structure determination. The intensive computations required in Hauptman's research will use the high performance computing resources of the Theory Center, which include one of the world's largest IBM RS/6000 POWERparallel System (SP).

The heart of the Parallel Resource is research led by Scheraga into the complexities of protein folding -- understanding how a polypeptide chain folds spontaneously into the three-dimensional form of a native protein.

The integration of new algorithmic approaches, combined with increasingly powerful computing resources, such as those provided in the Parallel Resource, promises dramatic results over the next decade, according to Scheraga. "We expect to be able to produce in the next few years at least as great an advance in the field as has occurred during the past 20 years," he said.

Biomedical scientists interested in accessing the Parallel Resource can find information about applying for time at: http://www.tc.cornell.edu/Allocations/.

Additional information about the Parallel Resource is at:

http://www.tc.cornell.edu/reports/NIH/resource/.

In addition to funding from NCRR at NIH, the Cornell Theory Center receives support from the National Science Foundation, New York State, IBM and members of the Theory Center's Corporate Partnership Program.

-30-