XXV.
Center for Information Technology

INTRODUCTION

The mission of the Center for Information Technology (CIT) is to provide, coordinate, and manage information technology and to advance computational bioscience at the National Institutes of Health (NIH).

CIT provides a vast array of information technology services to the NIH community, including networking, data center computing, enterprise applications development and support, computational bioscience and scientific computing, telecommunications, and user support and training. CIT also provides staff support to the Chief Information Officer of the NIH and performs the policy and oversight functions required by that role.

Working together, CIT's Divisions and the Office of the Deputy Chief Information Officer help to achieve the Center's goals. The five Divisions are the Division of Computational Bioscience, the Division of Computer System Services, the Division of Customer Support, the Division of Enterprise and Custom Applications, and the Division of Network Systems and Telecommunications.

CIT develops and provides the NIH backbone computer networking facilities and supports, guides, and assists other NIH components in local area networking. The Center provides professional programming services and computational and data-processing facilities to meet NIH program needs; operates and maintains the NIH Computer Center; designs and develops software; and provides extensive customer support, training courses and seminars, and documentation for computer and network users. CIT serves as the central systems analysis, design, and programming resource for data-processing and database projects relating to scientific, technical, management, and administrative data.

Guidance and support are provided to scientists and administrators throughout the NIH in the effective use of personal computers, workstations, local area networks, and associated automation technologies. CIT helps to coordinate, integrate, and standardize the vast array of computer services available throughout all of the organizations comprising the NIH.

The Center also serves as a scientific and technological resource for other parts of the U.S. Department of Health and Human Services and for other Federal organizations with biomedical, statistical, and administrative computing needs.

CIT promotes the application of high-performance computing and communication to biomedical problems, including image processing, structural biology, protein folding, database searching, gene-linkage analysis, and computational chemistry, by using advanced, massively parallel scalable computing. Computing technology is applied to research problems involving macromolecular structure representation and modeling and protein and DNA sequence analysis.

The CIT staff develops computer-based systems for laboratory and clinical applications, conducts computer science and engineering research and development, and consults and collaborates in computational, statistical, and mathematical aspects of data analysis. The staff also supports software systems to perform these analyses and conducts research in statistics and mathematics with applications to biomedicine.

As part of a separate role, the Center supports staff in the Office of the Deputy Chief Information Officer to develop a strong program for management of the NIH's information technology resources. This program includes putting processes in place to safeguard the confidentiality, integrity, and availability of automated information; to ensure that the NIH's information technology management program remains current with Federal requirements; and to develop policies and guidelines that are responsive to the NIH mission.

HIGHLIGHTS OF RECENT SCIENTIFIC ADVANCES RESULTING FROM INTERNATIONAL ACTIVITIES

CIT has assumed a major role in assisting the National Cancer Institute (NCI), NIH, in bringing the latest advances for the diagnosis and treatment of cancer to Ireland and Northern Ireland through its TELESYNERGY™ Medical Consultation WorkStation initiative. This multimodality medical teleconferencing environment, based at the NIH campus, is unique because of its ability to provide a synchronized, image-oriented environment to many participants at geographically distant sites.

CIT is assisting NCI by implementing the telemedicine component of the 5-year agreement among the governments of Northern Ireland, the Republic of Ireland, and the United States. This agreement is a historic Memorandum of Understanding, which combines the energies of the participants in the fight against cancer. The Memorandum of Understanding, signed by the three participating countries, directly specifies the use of "advanced telecommunications" to facilitate the joint cancer clinical trials initiative.

The TELESYNERGY™ System was demonstrated during the first NCI-All Ireland Cancer Consortium Conference, in Belfast, Northern Ireland, in October 1999. Because of the success of this demonstration, the medical teams in both Belfast, Northern Ireland, and Dublin, Republic of Ireland, intend that the TELESYNERGY™ System will be the telemedicine cornerstone of the Northern Ireland-Ireland-NCI Cancer Consortium.

Belfast City Hospital and St. Luke's Hospital, Dublin, are slated to have TELESYNERGY™ Systems installed during the second half of fiscal year 2001 (FY 01). NCI physicians and staff of the participating hospitals will be able to participate in clinic rounds, examine patients directly, review radiologic

and ultrasound data, and examine microscopic samples obtained through biopsy.

SUMMARY OF INTERNATIONAL PROGRAMS AND ACTIVITIES

Country-to-Country Activities and Bilateral Agreements

In FY 00, CIT scientists, investigators, and engineers successfully collaborated with scientists from a host of countries: Australia, Belgium, Canada, China, the Czech Republic, Egypt, France, Germany, Ireland, Israel, Japan, Jordan, Mexico, the Netherlands, Norway, Russia, Singapore, South Africa, Spain, Switzerland, and the United Kingdom. This international collaboration is exemplified through the TELESYNERGY™ System:

- An engineering manager from Singapore visited the TELESYNERGY™ System in January 2000.
- Medical staff from Belfast City Hospital, Northern Ireland, visited the TELESYNERGY™ System in February 2000.
- Physicians from Australia and Singapore visited the TELESYNERGY™ System in May 2000.
- Physicians from England, Germany, and Dublin, Ireland, visited the TELESYNERGY System in August 2000 and participated in a conference with staff members at another TELESYNERGY™ site—Holy Cross Hospital, Fort Lauderdale, Florida.

Two staff members from the CIT Division of Computational Bioscience (DCB) carried out site visits in August 2000 to the International Center for Cancer Treatment and Research, Brussels, Belgium, Belfast City Hospital, and St. Luke's Hospital, Dublin, to discuss the implementation of TELESYNERGY™ Systems at the three sites.

International Meetings

In FY 00, CIT scientists, investigators, and engineers participated in the following international meetings:

- DCB staff participated in the International Parallel Processing Symposium and the Symposium on Parallel and Distributed Processing, in Cancún, Mexico, in May 2000.
- A French Visiting Scientist from the Mathematical and Statistical Computing Laboratory (MSCL), DCB, organized the Bioinformatics Industrialization Workshop, which was held in Boston, Massachusetts, in June 2000. Another MSCL scientist attended this conference.
- DCB staff participated in the World Congress on Medical Physics and Biomedical Engineering, in Chicago, Illinois, in July 2000.
- A DCB scientist made a poster presentation entitled Trimethoprim Resistance in *Streptococcus pneumoniae:* Loss of a Single Hydrogen Bond Between Dihydrofolate Reductase and Trimethoprim, at the 2000 Computational Chemistry Gordon Research Conference, in Oxford, England, in July 2000.
- An MSCL scientist participated in the 8th International Conference on Intelligent Systems for Molecular Biology, in San Diego, California, in August 2000.
- Staff from the Bioinformatics and Molecular Analysis Section (BIMAS) of the Computational Bioscience and Engineering Laboratory (CBEL), DCB, participated in the FASEB (Federation of American Societies for Experimental Biology) Summer Research Conferences: Virus Assembly, at Saxton's River, Vermont, in the summer of 2000.
- BIMAS staff participated in the 12th European Congress on Electron Microscopy, Brno, Czech Republic, in the summer of 2000.
- An MSCL scientist attended the 12th International Genome Sequencing and Analysis Conference, at Miami Beach, Florida, in September 2000.
- An MSCL scientist presented an invited lecture on microArray data analysis at a conference entitled NanoBioTec, in Mhnster, Germany, in September 2000.
- Results of a collaboration to analyze the effect of a cancer drug on p53 knockout cells with a scientist from NCI were presented at an international meeting in Cairo, Egypt, in October 2000.
- An MSCL scientist presented a report at an international conference on Computers in Cardiology, in Boston, Massachusetts, in the fall of 2000.

Intramural Programs and Activities

BIMAS continues to be an official mirror site for the GeneCards database developed by the Weizmann Institute of Science, Rehovot, Israel.

In FY 00, BIMAS staff participated in an ongoing NCI-sponsored Lymphoma/Leukemia Molecular Profiling Project. The project is conducted by an international consortium including the British Columbia Cancer Agency; the University of Würzburg, Germany; the Norwegian Radium Hospital, Norway; and the University of Barcelona, Spain.

In addition, BIMAS staff met with visitors from the Netherlands Cancer Institute, who were on the NIH campus to review the microArray system developed by BIMAS for NCI.

Staff in the Image Processing Research Section worked on a number of joint studies to determine macromolecular structure by using images from electron microscopy. Of particular importance are the structure of selected viruses (herpes simplex virus, kshv, and bacteriophage T4), bacterial components, and other macromolecular structures. A Visiting Scientist from China is the chief electron microscopist in LSBR, National Institute of Arthritis and Musculoskeletal and Skin Diseases, NIH, and collaborates on many projects in structural biology. A Visiting Scientist from Japan cooperated in research to determine the three-dimensional structure of bacteriophage T4. Also, a Visiting Scientist from South Africa collaborated to investigate the structure of Kaposi's sarcoma virus and the maturation of herpes simplex virus type 1.

In MSCL, a Visiting Fellow from Spain completed studies of mathematical systems relevant to biophysical measurements.

An extensive collaboration to describe the gene expression profiles of cells of the immune system was undertaken by MSCL staff with a Visiting Fellow from China at the National Institute on Aging, NIH.

A Visiting Scientist from France worked in MSCL with investigators from NCI who are studying protein structure.

An MSCL scientist presented lectures related to single-molecule fluorescence spectroscopy at the University of Barcelona, Spain, and collaborated with a Spanish scientist. He also presented lectures at the Autonomous University of Mexico on single-molecule spectroscopy. In addition, the scientist worked with a professor at Bar Ilan University, Ramat Gan, Israel, on a problem related to optical imaging.

The collaborative efforts of DCB scientists and Visiting Professors were presented for review and publication in several instances. An article entitled "The net charge of the

first 18 residues of the mature sequence affects protein translocation across the cytoplasmic membrane of gram-negative bacteria" was published in the American Society of Microbiology's *Journal of Bacteriology* (April 2000). This publication was a result of research in the previous year. DCB scientists, in partnership with a Visiting Professor from the Institute of Biochemistry and Physiology of Microorganisms, Pushchino, Russia, had performed amino acid sequence analysis of signal peptides and the adjacent region, to explore the mechanism of protein translocation across the cytoplasmic membrane. The findings established that the net charge of the first 18 residues of the mature sequence is essential for protein translocation of gram-negative bacteria.

In October 2000, Elsevier Science Ltd.'s *Trends in Biochemical Sciences* published a review entitled "When protein folding is simplified to protein coiling: the continuum of solenoid protein structures" (volume 25). The review, which was written jointly by DCB staff and Visiting Professors from Australia and Russia, summarized a DCB study to obtain data about the activity of superhelical or solenoid structures. The research centered on classification of these structures and characterization of the general features of solenoid structures.