Bioinformatics Workshop

Biomedical Research Infrastructure Networks (BRIN) and Research Centers in Minority Institutions (RCMI) National Center for Research Resources (NCRR) National Institutes of Health (NIH) March 8 - 9, 2002

Los Alamos Research Park Conference Center Los Alamos National Laboratory (LANL) Los Alamos, New Mexico

Organizers and Speakers:

Bob Boehmer, Informax, Incorporated

Howard Cash, Gene Codes Corporation

Kevin Facemyer, Ph.D., Nevada BRIN Director of Planning and Education, University of Nevada, Reno

David Forslund, Ph.D., Laboratory Fellow, LANL

Paul Gilna, Ph.D., Scientific Thrust Coordinator, Bioscience Division, LANL

Susan R. Kayar, Ph.D., BRIN Coordinator, Health Scientist Administrator, NCRR, NIH Kevin Kendall, Accelrys

Shelia McClure, Ph.D., RCMI Coordinator, Health Scientist Administrator, NCRR, NIH Sidney A. McNairy, Jr., Ph.D., D.Sc., Associate Director for Research Infrastructure, NCRR, NIH

William Southerland, Ph.D., Professor of Biochemistry, Howard University

Karl Steiner, Dr. Ing., Associate Director, Delaware Biotechnology Institute, University of Delaware

Juarine Stewart, Ph.D., Professor of Biology, Clark Atlanta University

Jennifer Weller, Ph.D., Research Assistant Professor, Adjunct Assistant Professor of Biology, Virginia Bioinformatics Institute

David Wheeler, Ph.D., Staff Scientist, National Center for Biotechnology Information, National Library of Medicine, NIH

Friday, March 8, 2002

Welcome and Introduction to LANL

Dr. Forslund expressed his pleasure that the participants could avail themselves of the LANL conference facility. Dr. McNairy welcomed the BRIN and RCMI participants on behalf of the NCRR. He commended them for being at the forefront of helping people through biomedicine, and for educating the scientific leaders of the future. He described how the impetus for this event came from the Institutional Development Award (IDeA) program meeting in Oklahoma City in October 2001, where he recruited Drs. Steiner, Facemyer, and others to develop a bioinformatics workshop. He congratulated the organizers on their success, and expressed his hope that the participants would profit from the partnerships they forged here. Dr. Facemyer thanked participants for making the effort to travel to such a distant place. He expressed his pleasure in

participating in the BRIN program as a means of renewing hope. Dr. Steiner described the combined BRIN/RCMI workshop as an opportunity to build programs that would be scientifically and culturally richer because of these interactions. He described forming a network of multiple institutions as difficult but essential in building for the future.

The Importance of Distributed, Component-Based Healthcare Information Systems: The Role of a Service-Based Architecture

Dr. Forslund explained that the impetus for Internet2 comes from the inability of the current Internet to deal with millions of users, multimedia, or real-time interactions. Internet2 is designed for distributed computation, virtual laboratories, digital video, and other high-throughput uses. In assessing their computer needs, researchers must plan for interactions with others to assure that their approaches are compatible. Some important Web sites that may be beneficial to workshop participants as they plan ahead are:

- http://www.omg.org/
- http://openEmed.org/
- http://www.semanticweb.org/

Collaboratories Demonstration

Dr. Steiner presented a live demonstration of remote access to a bioimaging facility over a Webbased network. A computer at the workshop was linked to a laboratory at the Delaware Biotechnology Institute (DBI), where Dr. Kirk Czymmek, Associate Professor in Biological Sciences at DBI (Kirk@udel.edu), was operating a multi-photon confocal microscope and generating images of surface structures on a wasp. Dr. Czymmek appeared on a video screen with audio connection, along with the images he was examining. Using this high-throughput connection, workshop participants were able to ask him questions about the preparation and direct him toward preferred images. These images could be archived for future retrieval. This system makes it possible to collaborate with anyone in the world with compatible software and adequate Internet connection speed. Costs, software, and hardware needs were discussed.

Saturday, March 9, 2001

BRIN and **RCMI** Bioinformatics Activities

Participants shared three-minute summaries of their bioinformatics activities and provided opportunities for questions and discussion. Activities at each institution were compared to the <u>diagrammatic overview of bioinformatics</u> devised by Cynthia Gibas and Per Jambeck. Prior to the workshop, participants were asked to submit one-page executive summaries of the goals, approaches and challenges for implementing the bioinformatics core at their BRIN or RCMI program. <u>These summaries</u> were made available to the workshop participants to facilitate matching of core interests.

Bioinformatics Perspectives: Expert-Led Discussions of Issues and Solutions

Integration, integration, and integration are the three most important aspects of bioinformatics, according to Dr. Gilna. The former "reductionist" view of biology is now being replaced by a "constructionist" phase, in which the interface between biology and computers is a critical element. The biological scientists and computer scientists must work together to achieve critical mass, to increase the breadth of research that can be performed, and to solve the problems of "software hardening" in which tools designed in one environment must be used in another. Dr. Gilna reminded the audience that future Federal budgets for biomedical research would depend on the success of their current efforts.

Dr. Weller described the bioinformatics services available from her institution. One can send them a genomic database, which they filter for input errors and analyze. She gave a live, on-line demonstration of the steps involved in registering a project and initiating an analysis.

The panel members spent 20 minutes each to introduce their topics, and then the floor was opened for questions and discussion. Topics discussed included: methods for cleansing databases; flexibility of analyses; the critical role of statisticians and mathematicians in biological projects; and the difficulty of recognition and promotion for faculty who are spending time on writing software or analyzing others' data, rather than writing research papers.

Bioinformatics Tools and Training

Representatives of three software vendors (Accelrys, Gene Codes, and Informax) were present throughout the workshop and available for informal conversations with participants. A panel, composed of one representative from each vendor (Kevin Kendall, Howard Cash, and Bob Boehmer) was assembled, with each representative making a presentation of 20-30 minutes. They discussed some of the issues regarding bioinformatics tools and data management from the perspective of their respective companies. The floor was then opened for discussion. Questions centered on costs of software and training; ability to negotiate group discounts; user friendliness of products; and willingness of companies to incorporate algorithms developed by university users. Finally, some examples of the use of genomics in forensic science were described.

Developing Biome dical Research Programs

Administering bioinformatics programs, training bioinformatics experts, attracting qualified graduate students, assessing needs, setting program priorities, and securing resources were among the topics assigned to Dr. Southerland and Dr. Stewart. Dr. Southerland described the keys to growth of a bioinformatics program as scientific versatility and convenience. Securing service contracts for machines, purchasing hardware upgrades, and hiring qualified personnel are the biggest challenges to maintaining bioinformatics core needs.

Dr. Stewart, who is President of the RCMI Program Directors' Association, recommended http://www.biology.gatech.edu/bioinformatics as a useful source of information on bioinformatics. This is the Web site for the Master's Degree program in bioinformatics at Georgia Institute of Technology, the nation's first such program. With growing numbers of students receiving their information technology training through science programs such as this one, it will become easier to fill science department faculty slots, rather than seeing all the most

technically-adept high school students recruited by industry. Summer internships, graduate programs in bioinformatics, and competitive stipend packages will all help attract qualified graduate students. Securing resources is an ongoing process for which all avenues must be continually pursued. Scientists cannot afford to isolate themselves in their labs, only performing research. Setting priorities, establishing an agenda for meeting the priorities, and identifying people with key responsibilities for each activity are crucial.

Courses, Training and Outreach Programs

Dr. Wheeler indicated that computerized bioinformatics is such a new field that most biologists have little familiarity with it. The National Library of Medicine (NLM) is prepared to help with this problem by offering a variety of courses via the Internet, in person at the NLM, or on request at outside institutions. Many of these courses are free of charge. It was suggested that participants should see the NLM home page. They have provided training for using software for genomics and proteomics research, and many others.

The workshop program concluded with summaries and thanks from the coordinators. Questions about the meeting may be addressed to Dr. Karl Steiner (Steiner@dbi.udel.edu), Dr. Kevin Facemyer (Facemyer@unr.edu), Dr. Susan Kayar (KayarS@ncrr.nih.gov), or Dr. Shelia McClure (McclureS@ncrr.nih.gov). A more detailed summary of the workshop, including executive summaries from participants, PowerPoint presentations of speakers, and some photographs of meeting activities, appears at the University of Delaware Web site at which participants registered. The University of Puerto Rico has also made available a summary of the meeting that includes photographs of participants.