The Conception, Gestation, and Birth of the National Centers for Biomedical Computing

Eric Jakobsson
University of Illinois at Urbana-Champaign
National Center for Supercomputing Applications
Director, NIH Roadmap National Center for the Design of Biomimetic Nanoconductors
Former Chair, NIH Biomedical Information Science and Technology Initiative Consortium

For: CSB 2006

August 15, 2006

Why Computational Biology at the NIH

- Because computation and information technology is an invaluable tool for understanding biological complexity, which is at the heart of advance in biomedical knowledge and medical practice.
- “You can’t translate what you don’t understand”---Elias Zerhouni, Director of the National Institutes of Health, commenting on the relationship between basic research and translational research, that transforms the results of basic research into a foundation for clinical research and medical practice.

Some important problems with biomedical computing tools:

- They are difficult to use.
- They are fragile.
- They lack interoperability of different components
- They suffer limitations on dissemination
- They often work in one program/one function mode as opposed to being part of an integrated computational environment.
- There are not sufficient personnel to meet the needs for creating better biological computing tools and user environments.

Why the problems with biological computing tools must be fixed.

- Today computation is at the heart of all leading edge biomedical science. For leading examples, consider recent Nobel prizes:
- Structure of voltage-gated channels—required sophisticated computation for image reconstruction for x-ray diffraction data, the mathematical techniques for which were the subject of a previous Nobel prize.
- Discovery of water channels—The experimental work required augmentation by bioinformatics for identification of water channel genes by sequence homology.
- Magnetic resonance imaging—A large share of the prize work was for the mathematical and computational techniques for inferring structure and image from nmr spectra.

The Paradox of Computational Biology--Its successes are the flip side of its deficiencies.

- The success of computational biology is shown by the fact that computation has become integral and critical to modern biomedical research.
- Because computation is integral to biomedical research, its deficiencies have become significant rate limiting factors in the rate of progress of biomedical research.

Mission Statement (stated in 2004)

- In ten years, we want every person involved in the biomedical enterprise---basic researcher, clinical researcher, practitioner, student, teacher, policy maker---to have at their fingertips through their keyboard instant access to all the data sources, analysis tools, modeling tools, visualization tools, and interpretative materials necessary to do their jobs with no inefficiencies in computation or information technology being a rate-limiting step.

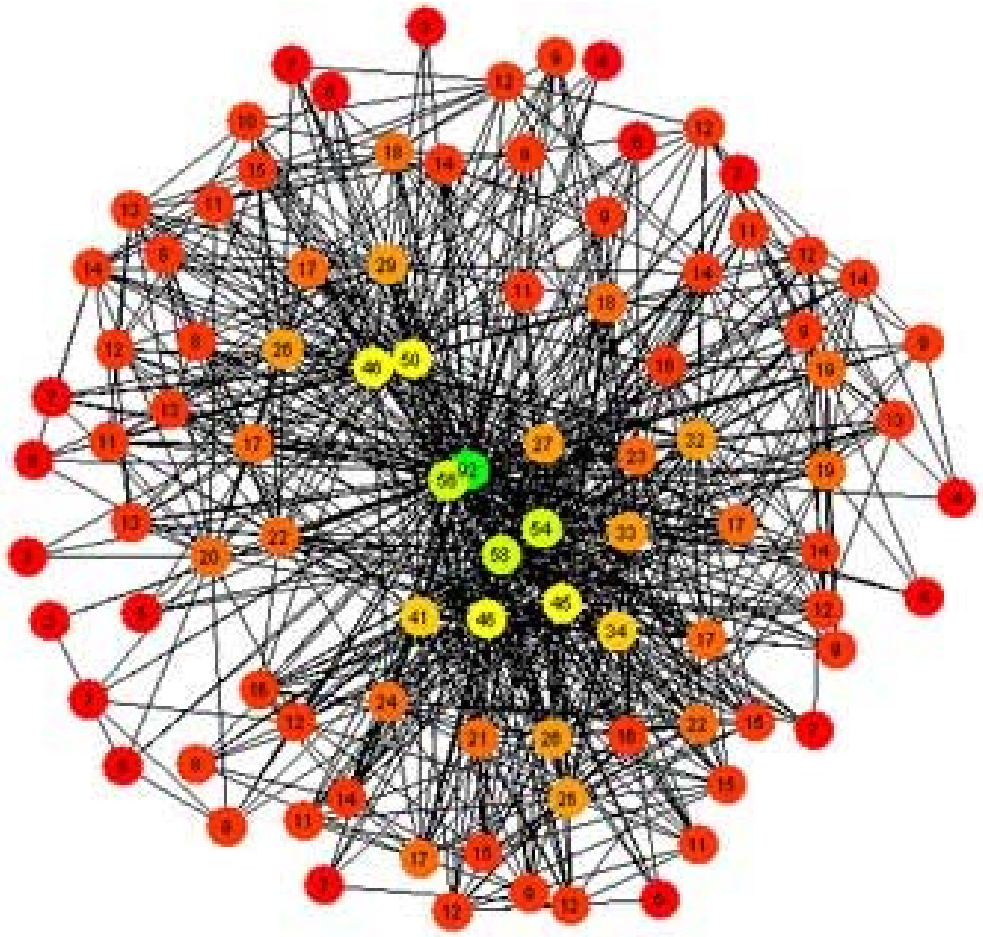
Computational Biology at the NIH—why, whence, what, whither. ---Whither: The NIH Bioinformatics and Computational Biology Roadmap:

- Was submitted to NIH Director Dr. Elias Zerhouni on May 28, 2003
- Was the outline of an 8-10 year plan to create an excellent biomedical computing environment for the nation.
- Had as its explicit most ambitious goal “Deploy a rigorous biomedical computing environment to analyze, model, understand, and predict dynamic and complex biomedical systems across scales and to integrate data and knowledge at all levels of organization.

NCBC's---the heart of the Roadmap for Biomedical Computing

- Each Center is to serve as a node of activity for developing, curating, disseminating, and providing relevant training for, computational tools and user environments in an area of biomedical computing.
- The PI's of the Centers are called not to glory, but to service

A scale free---or semi-scale free---network, simultaneously internally robust and adaptive to changing circumstance—NCBC's envisaged to be the highly connected nodes at the center. Instead of having big science and small science compete with each other, we intended to create an environment in which they will work hand in hand for the benefit of *all* science**.**



SOME CHALLENGES IN BIOMEDICAL COMPUTING AS DEFINED BY BIOMEDICAL CONTENT

1. In silico screening of drug compounds.
2. Predicting function from structure of complex molecules at an engineering level of precision.
3. Accurate, efficient, and comprehensive dynamical models of spread of infectious disease.
4. Integration of the computational tools of systems biology into an integrated computational environment for information-based modeling of pathways, networks, cells, and tissues.
5. Computerization of the health care delivery system.
6. Prediction of protein structure to the point where all protein sequences have associated accurate structures.
7. Complete annotation of the genomes of selected model organisms.
8. Intelligent systems for mining biomedical literature
9. Tuning biomedical computing software to hardware.
10. Utilizing computational biology tools in education
11. Computer-aided design of biomimetic devices.
12. Realizing the potential of personalized medicine.

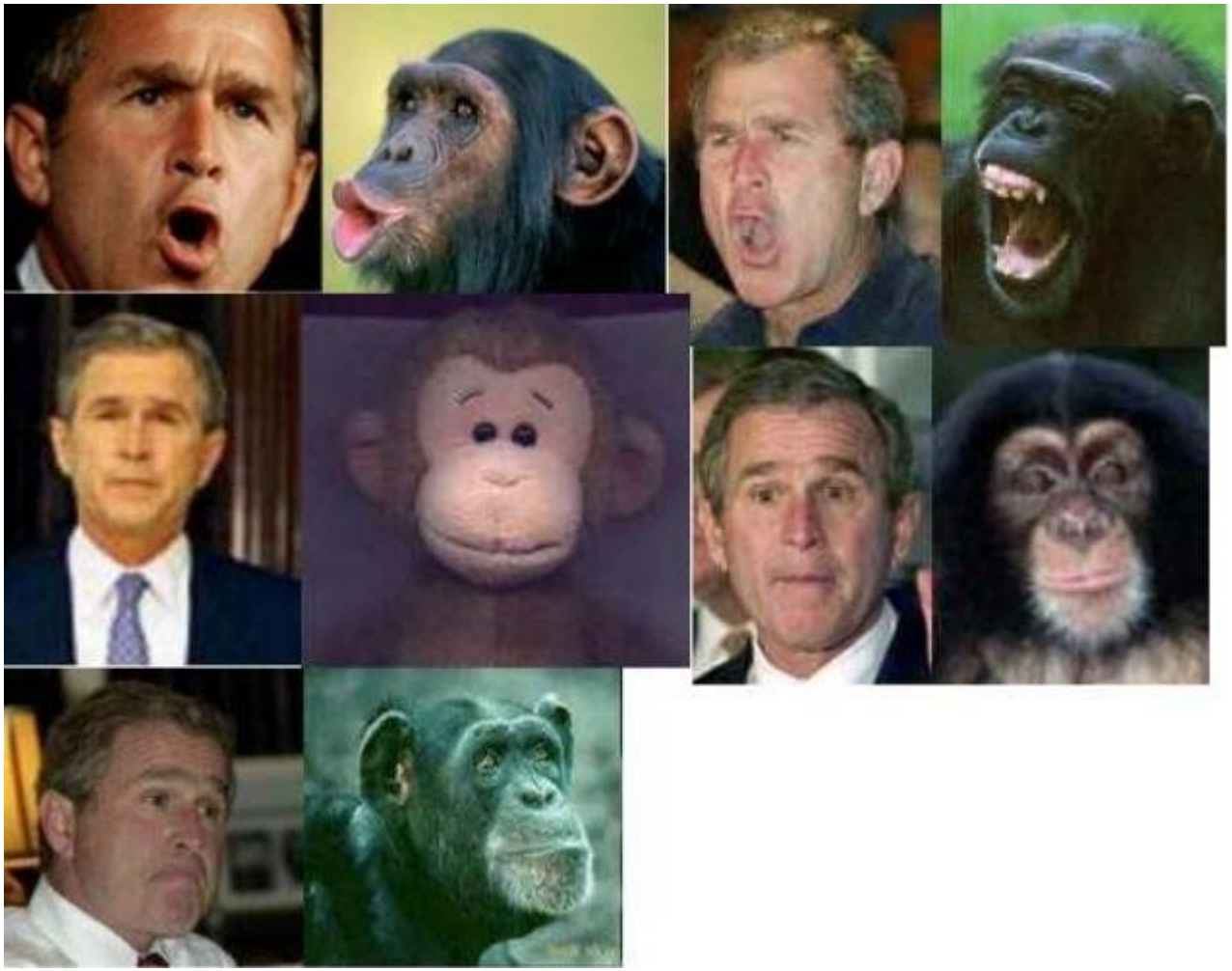
CHALLENGES IN BIOMEDICAL COMPUTING AS DEFINED BY HIGH LEVEL COMPUTING STRATEGY.

- Integration of time and length scales of description.
- Integration of informatics, dynamics, and physical-based approaches.
- Integration of literature with other data forms.
- Integration of basic science with engineering design.
- Integration of algorithmic development with computing architecture design.
- Putting the new computational biology workforce in place.

Major Problems in American Education

- We are not training American biology researchers with quantitative skills at even close to a rate to sustain, let alone advance, American biology.
- A large number of Americans are fundamentally ignorant about biology, both in practical and theoretical terms. For example, about 50% of Americans do not believe in evolution….

…In spite of the obvious evidence; i.e., "The relative position of our features is manifestly the same; and the various emotions are displayed by nearly similar, movements of the muscles and skin, chiefly above the eyebrows and round the mouth."----Charles Darwin, *The Descent of Man*



Take-Home Lessons (Cliches, but true)

- Tend to the details, but keep the big picture in mind—we are working on really important stuff.
- Amid all of the bureaucrap, try to remember why you decided to become a scientist in the first place—”Hold fast to the spirit of youth, let years to come do what they may.””---on a mantelpiece in a dormitory at Columbia University.