

What do biologists need to compute?

Bob Elde, Dean
College of Biological Sciences and
Professor, Department of Neuroscience

- “Computation, driven in part by the influx of large amounts of data at all biological scales, has become a central feature of research and discovery in the life sciences.” Bourne, Brenner & Eisen, PLoS Computational Biology 1:1, 2005

- “Computational biology thrives on open access to DNA sequences, protein structures and other types of biological data. . .” *ibid*

Historical examples of computation in biology

- Hodgkin-Huxley modeling of membrane potential and action potential
- Kinetic analysis of enzymes, receptor/ligand interactions
- Development as the French flag problem
- Ecosystem sciences

Converging opportunities

- “. . .from molecules to ecosystems.”

Computer Simulation in Biology, Keen &
Spain, 1992

Table of Contents - Simple Model Equations

- Analytical models based on differential equations
- Analytical models based on stable states
- Estimating model coefficients from experimental data
- Planning and problems of programming
- Numerical solution of rate equations

Models with multiple components, Keen & Spain, 1992

- Kinetics of biochemical reactions
- Models of homogeneous populations of organisms
- Simple models of microbial growth
- Population models based on age-specific events
- Simulations of population genetics
- Models of light and photosynthesis
- Temperature and biological activity

Multiple components, Keen & Spain, 1992 - continued

- Compartmental models of biogeochemical cycling
- Diffusion models
- Compartmental models in physiology
- Application of matrix methods to simulations
- Physiological control systems

Probabilistic models, Keen & Spain, 1992

- Monte Carlo modeling of simple stochastic processes
- Modeling of sampling processes
- Random walks and related stochastic processes
- Markov chain simulations in biology

Supplementary models, Keen & Spain, 1992

- Models of cellular function
- Models of development and morphogenesis
- Models of epidemics

Computation in the curriculum

- Take calculus
- Statistics for the disinterested scientist

Genomics - Bioinformatics

- Data mining
- Pattern recognition

Proteomics

- Data mining
- Higher order modeling of structures
- Pattern recognition

Metabolomics

- Flux through all pathways under all conditions

- Cellomics
- Higher order function
- Systems biology

Examples

- Center for Cell Dynamics
<http://raven.zoology.washington.edu/celldynamics/>
- Bacterial chemotaxis
<http://flash.uchicago.edu/~emonet/biology/agentcell/>
- Imaging
<http://images2.aperio.com/aperio/view.apml?cwidth=852&cheight=535&chost=images2.aperio.com&returnurl=http://www.aperio.com/&csis=0>

What do we need, here and
now?

Put the needs of our students first, and
everything else will fall into place,
almost naturally (after Donald Kennedy, *Academic
Duty*)