



NSDL/NSTA Web Seminar:
Computational Biology



Tuesday, December 11, 2007
6:30 p.m. - 8:00 p.m. Eastern time



Agenda:

1. Introductions
2. Tech-help info
3. Web Seminar tools
4. Presentation
5. Evaluation
6. Chat with the presenter

Supporting the NSDL Presenting Team are...

For additional Tech-help call:

Illuminate Support,

1-866-388-8674 (Option 2)



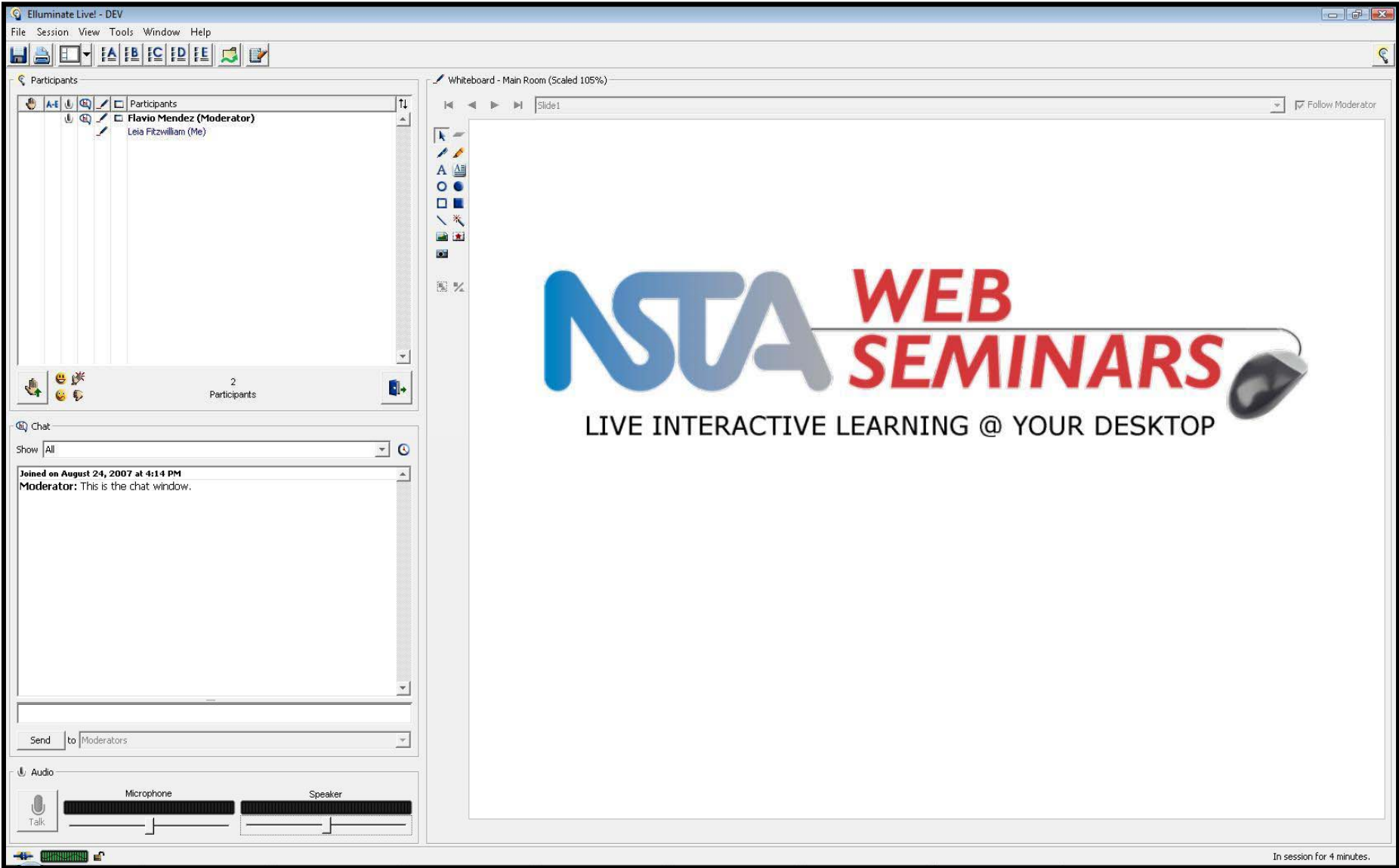
Jeff Layman
Tech Support, NSTA
jlayman@nsta.org
703-312-9384



<http://nsdl.org>



Screenshot





We would like to know more
about you...

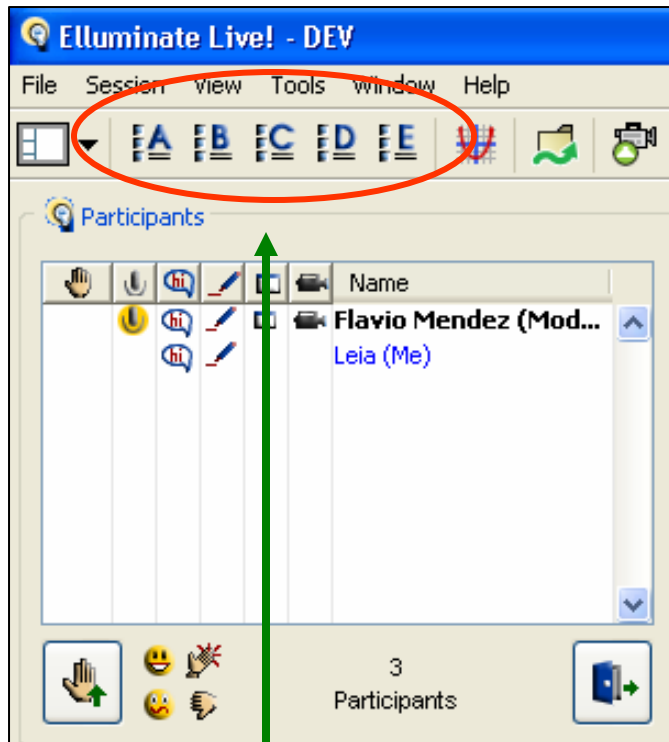


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How many web seminars have you attended?



A. 1-3

B. 4-5

C. More than 5

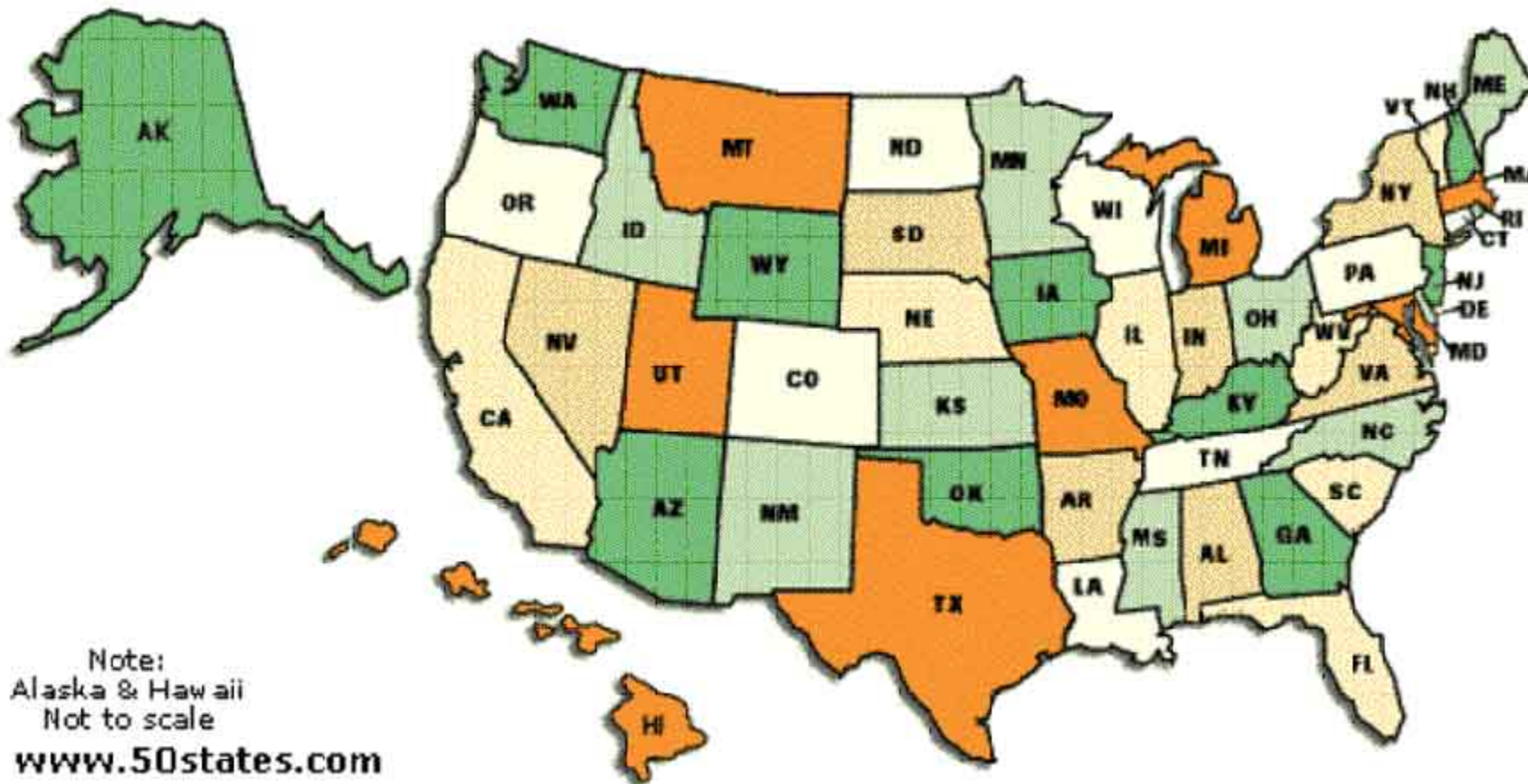
D. More than 10

E. This is my first web seminar

Use the letters A-E located at the top left of your actual screen to answer the poll



Where are you now?



Note:
Alaska & Hawaii
Not to scale
www.50states.com



<http://nsdl.org>





What grade level do you teach?



- A. Elementary School, K-5.
- B. Middle School, 6-8.
- C. High School, 9-12.
- D. I teach undergrad and/or grad students.
- E. I am an Informal Educator.



NSDL/NSTA Web Seminar:
Computational Biology



Tuesday, December 11, 2007



Today's NSDL Expert:



Dr. Jeff Krause
Staff Computational Biologist and Educator
Shodor Foundation, Inc



<http://nsdl.org>



<http://www.shodor.org>



<http://cserd.nsdl.org>



<http://www.nsta.org>



Agenda

- **Introduction**
- **Background on contemporary (computational) biology**
- **Protein structure and molecular motion**
- **Protein networks and systems biology**
- **Tools for teaching system thinking**




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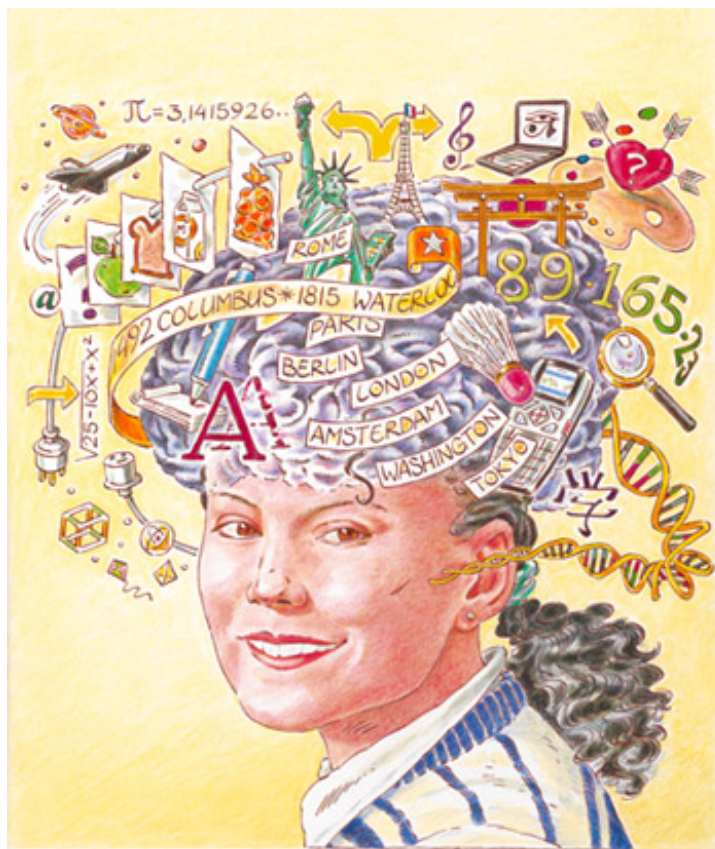


Stamp all the categories that apply to you. I teach....

Biology	Math	General Science
Computation/ Programming	None of these	
		

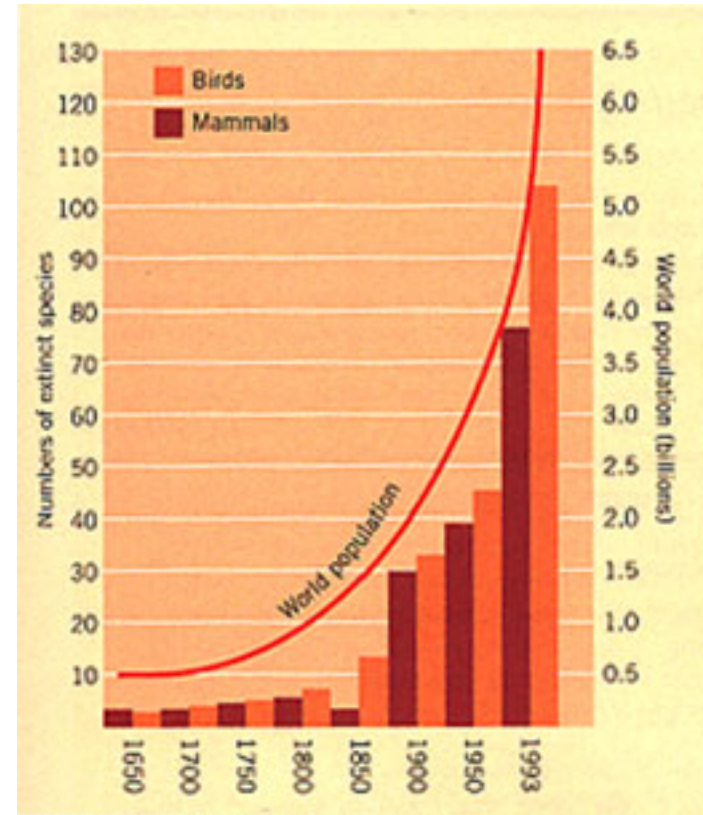
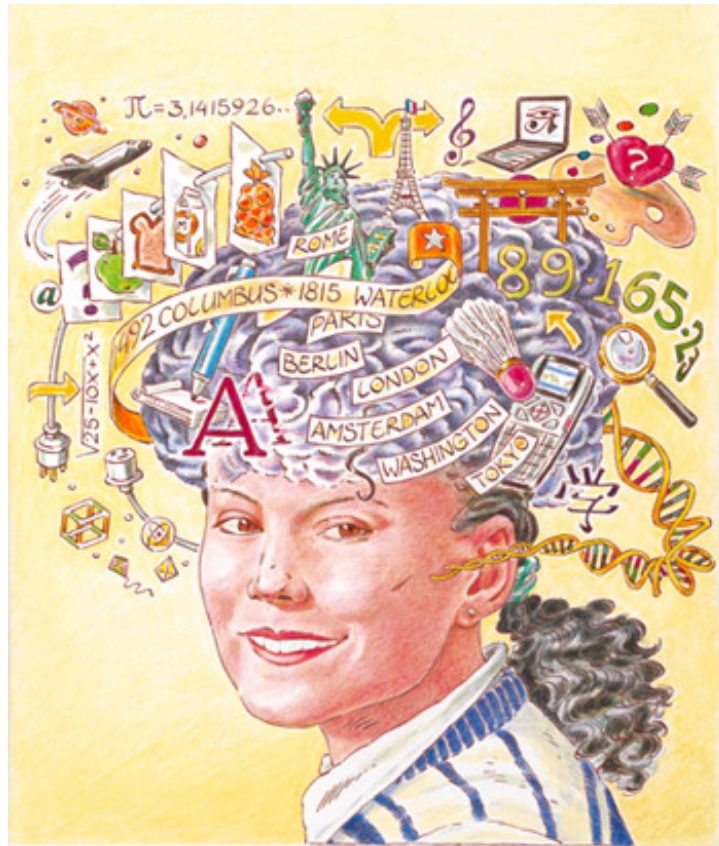


Introduction: My Neuro-Computational Perspective





Introduction: My Neuro-Computational Perspective



Source: Dr. Richard A. Bradley,
Associate Professor, Biology, Ohio State University



<http://nsdl.org>



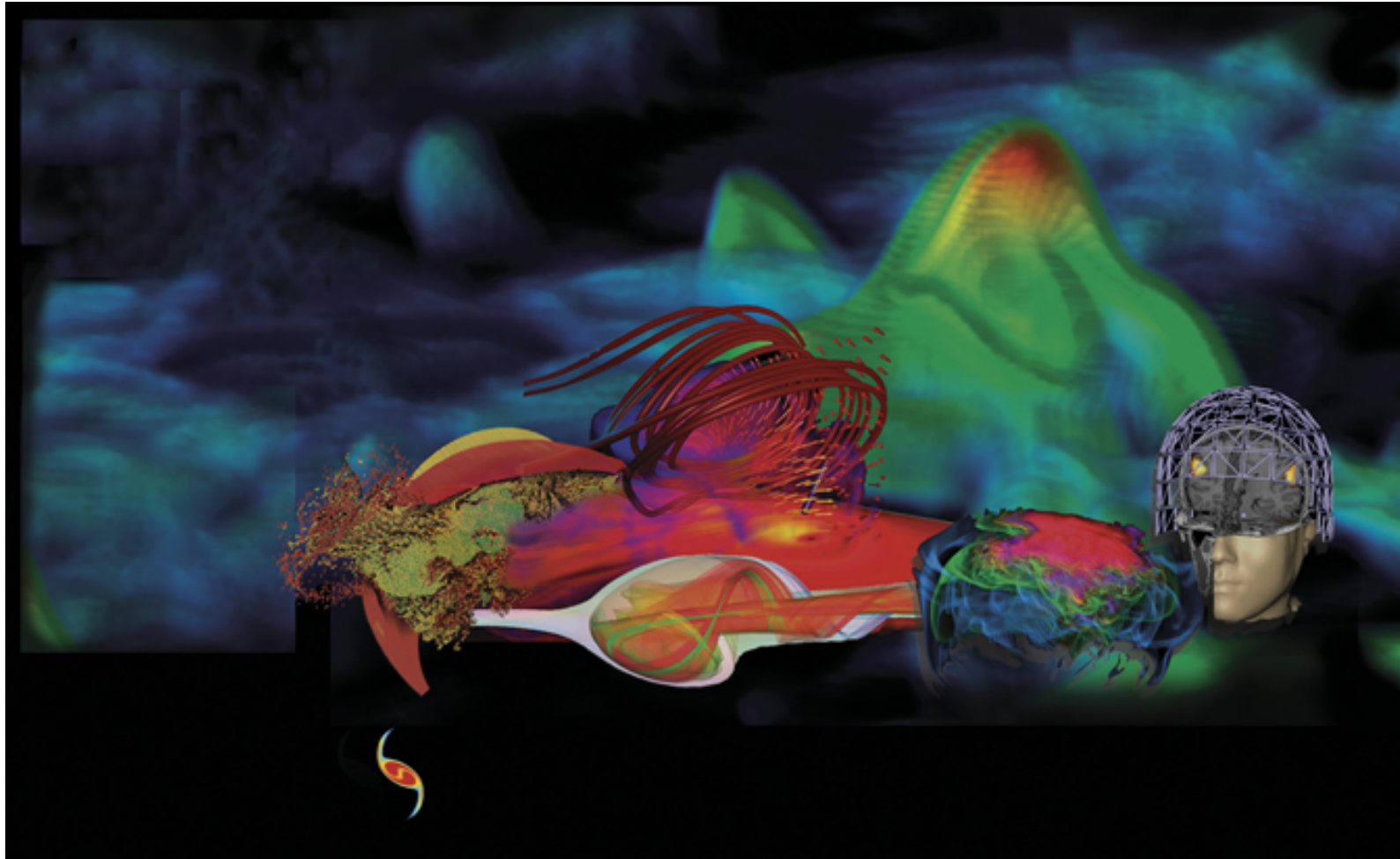


Introduction: My Neuro-Computational Perspective





Introduction: My Neuro-Computational Perspective



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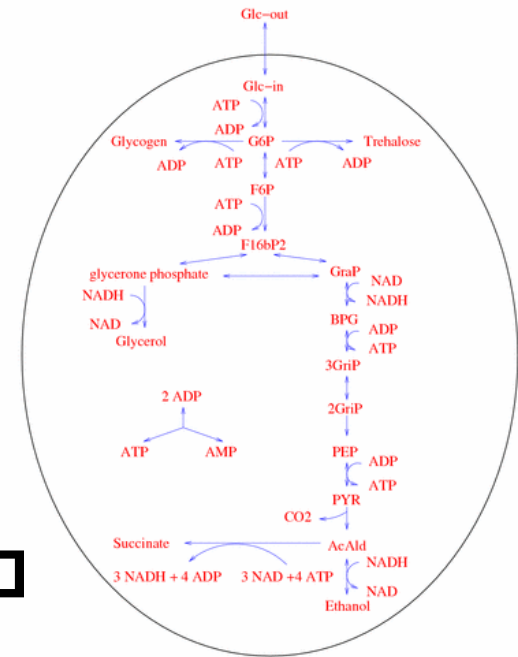
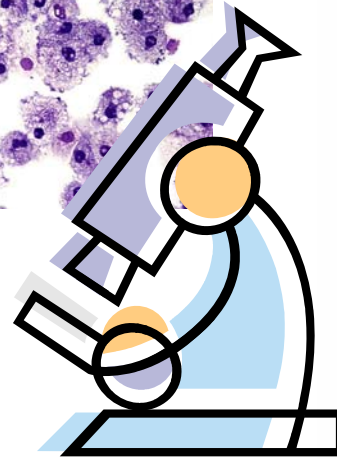
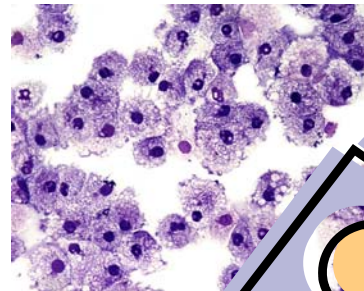




Contemporary Biology: A short history



Biology as a
“hard” science

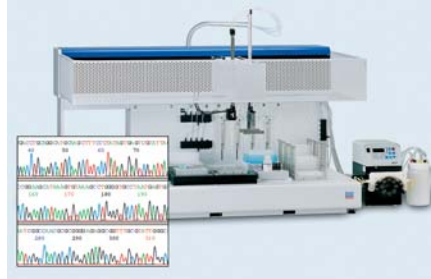


Use reductionism to
deal with biological
complexity





Contemporary Biology: A short history



High-throughput biomolecular measurement technologies and the “genomic revolution”

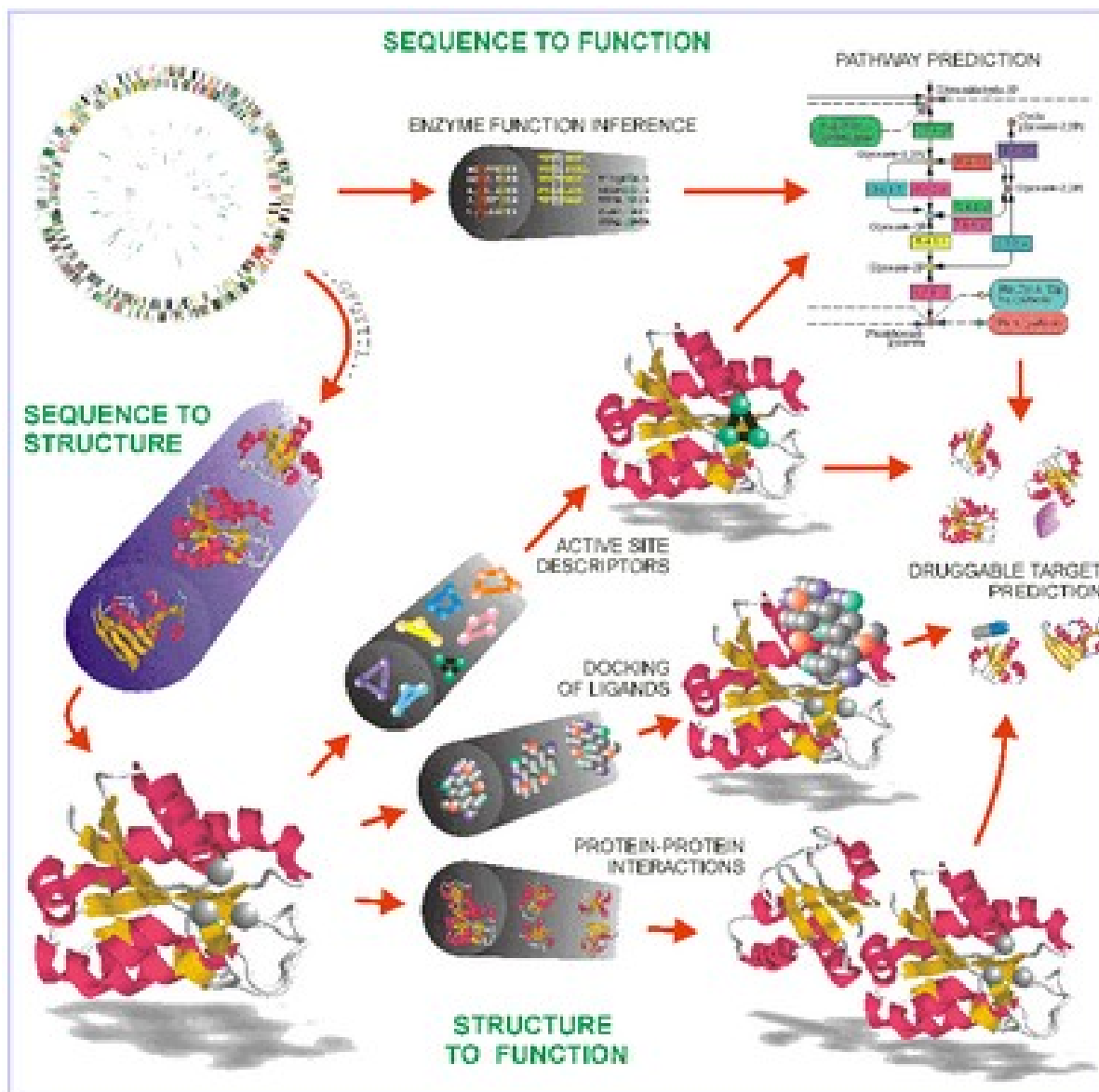


<http://nsdl.org>





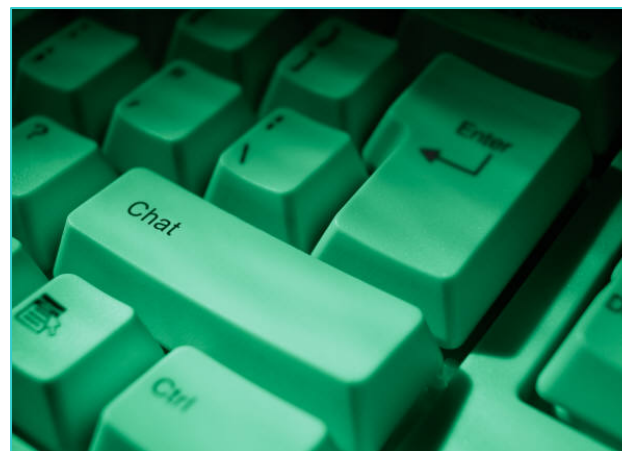
Contemporary Biology: A short history





The molecular world is unintuitive to most students (and teachers). How does the molecular world differ from our everyday experience?

Write your ideas
on the chat





The Molecular Literacy Project

<http://molit.concord.org>

The screenshot shows a web browser window with the URL <http://molit.concord.org/>. The page features a navigation menu with links for Home, Database, News, Software, Research, and Authoring. A search bar is present with the text "Search the Database: enter keywords" and a "Go" button. There are also buttons for "Jump to Activity: # Student Teacher". The Molecular Literacy logo is prominently displayed.

This project is a continuation of the work on the [Molecular Workbench project](#) and the [Molecular Logic project](#)

The Molecular Literacy Project

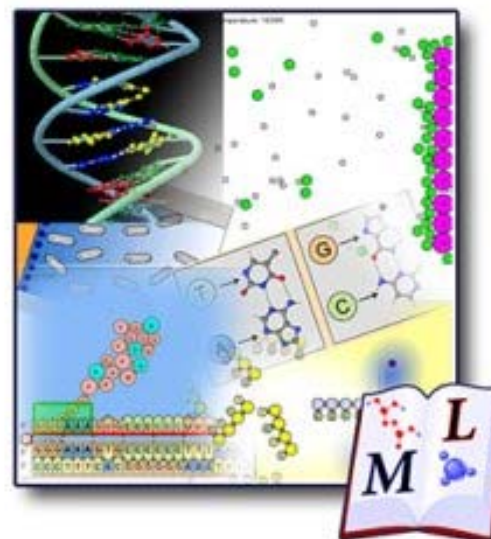
This three-year project worked to enhance science and technology teaching in grades 10-14 by providing Molecular Literacy content in support of careers in biotechnology and nanotechnology. The project developed new materials that used highly interactive molecular dynamics and quantum mechanics models, and embed these models in learning activities that are appropriate for both core science courses and specialized courses teaching biotechnology and nanotechnology workplace competencies. In developing these materials, the Concord Consortium worked with its partner, Middlesex Community College, Bedford, Massachusetts, as well as its feeder high schools, additional community colleges (including Roxbury Community College, Parkland College, and Wachusett Community College), biotechnology and nanotechnology companies, and COD, an educational non-profit in Texas, which provided national dissemination.

[MoLit Project Final Report](#)

[Core MoLit Activities at a Glance](#)

[View Our Database Activities](#)

[Read Project News](#)

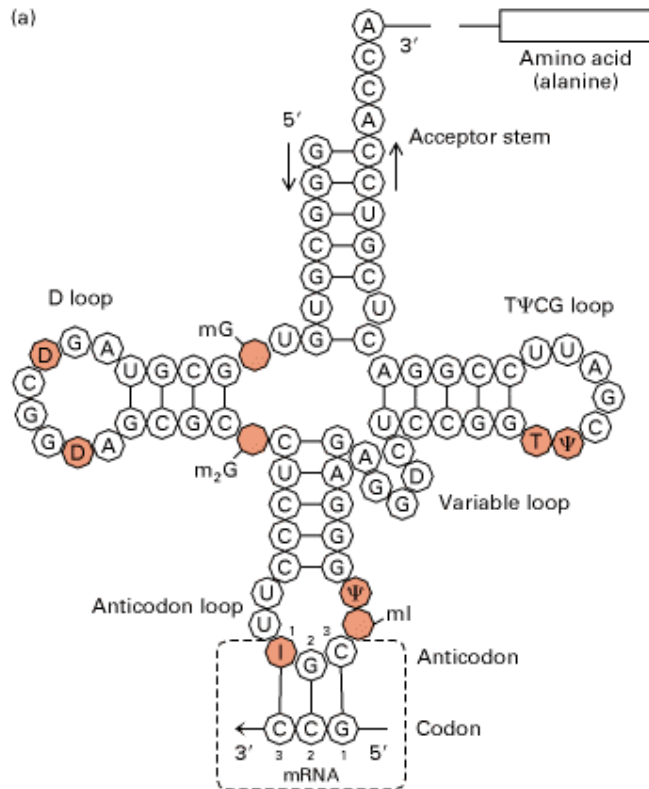


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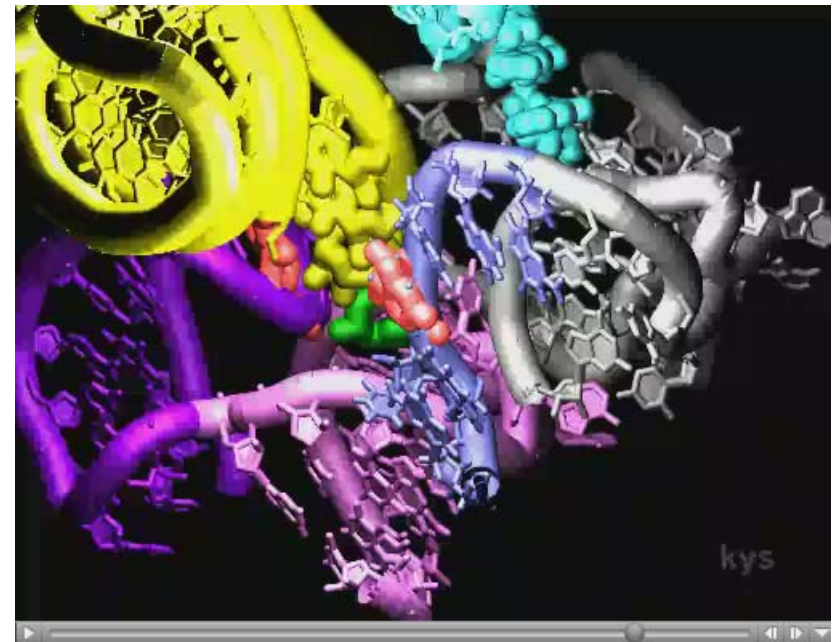




Seeing Real Protein Structure, Function and Dynamics



Typical textbook
molecular structure



Molecular dynamics
simulation



The Protein Data Bank

<http://www.rcsb.org/pdb>

Are you missing data updates? The PDB archive has moved to <ftp://ftp.wwpdb.org>. For more information click [here](#).

Welcome to the RCSB PDB

The RCSB PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease.

The RCSB is a member of the [wwPDB](#) whose mission is to ensure that the PDB archive remains an international resource with uniform data.

This site offers tools for browsing, searching, and reporting that utilize the data resulting from ongoing efforts to create a more consistent and comprehensive archive.

Information about compatible browsers can be found [here](#).

A [narrated tutorial](#) illustrates how to search, navigate, browse, generate reports and visualize structures using this new site. [This requires the [Macromedia Flash player](#) download.]

Comments? info@rcsb.org

Molecule of the Month: Oxidosqualene Cyclase

Cholesterol has gained a bad reputation in recent years. It is absolutely

News

- Complete News
- Newsletter
- Discussion Forum

04-December-2007

Announcement: Experimental Data Will Be Required for Depositions Starting February 1, 2008

Effective February 1, 2008, structure factor amplitudes/intensities (for crystal structures) and restraints (for NMR structures) will be a mandatory requirement for PDB deposition.

- Full article ...

27-November-2007

RCSB PDB Focus:



<http://nsdl.org>





Additional Collections for Protein Structure and Dynamics....

Go to the NSDL K-12 page
resource list for this seminar

http://nsdl.org/resources_for/k12_teachers



<http://nsdl.org>





VMD: Visual Molecular Dynamics

THEORETICAL *and* COMPUTATIONAL
BIOPHYSICS GROUP

NIH RESOURCE FOR MACROMOLECULAR MODELING AND BIOINFORMATICS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Home
Overview
Publications
Research
Software
VMD Molecular Graphics Viewer
NAMD Molecular Dynamics Simulator
BioCoRE Collaboratory Environment
MD Service Suite
Structural Biology Software Database
Computational Facility
Outreach

VMD Community Pages

Download VMD

VMD Tutorials

VMD

VMD
Visual Molecular Dynamics

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS-X, Unix, or Windows, is distributed free of charge, and includes source code.
[\(more details...\)](#)

Spotlight

"I would add that VMD (and similar tools, if they yet exist) will become a primary platform upon which to study a wide range of biological problems in the future. VMD adds a new dimension to the biologist's thinking. Certain thoughts generated in interaction with VMD images are inconceivable otherwise; the 'language' essential to generating these ideas would just not be there! In other words, VMD is far from a simple 'visualization tool' for a biologist, it is a true thinking tool. Without it a whole class of biological hypotheses would simply not exist."
-- Carl Woese



<http://nsdl.org>

<http://ks.uiuc.edu/research/vmd>





How many of you have seen or used any of these tools before?

- A. I haven't seen or used them before
- B. I knew about some of them as research resources but not educational resources
- C. I have used them in class to positive effect
- D. I have used them in class but they weren't helpful

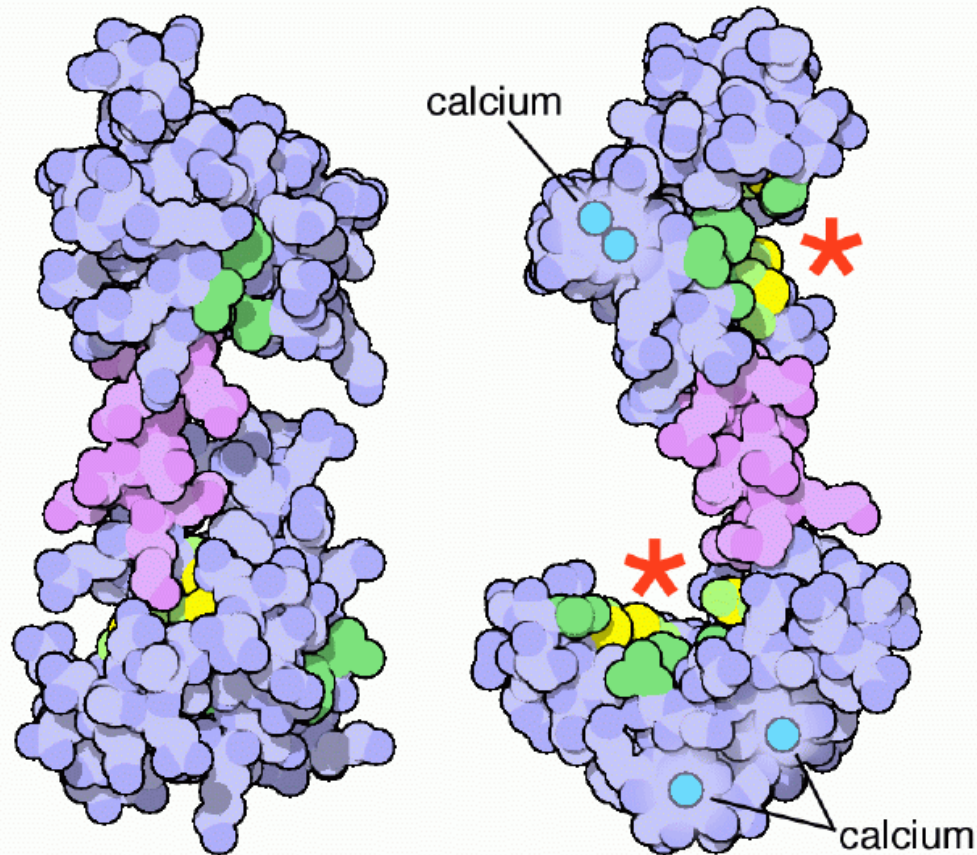


<http://nsdl.org>





An Example: Calcium-Induced Structural Change in Calmodulin



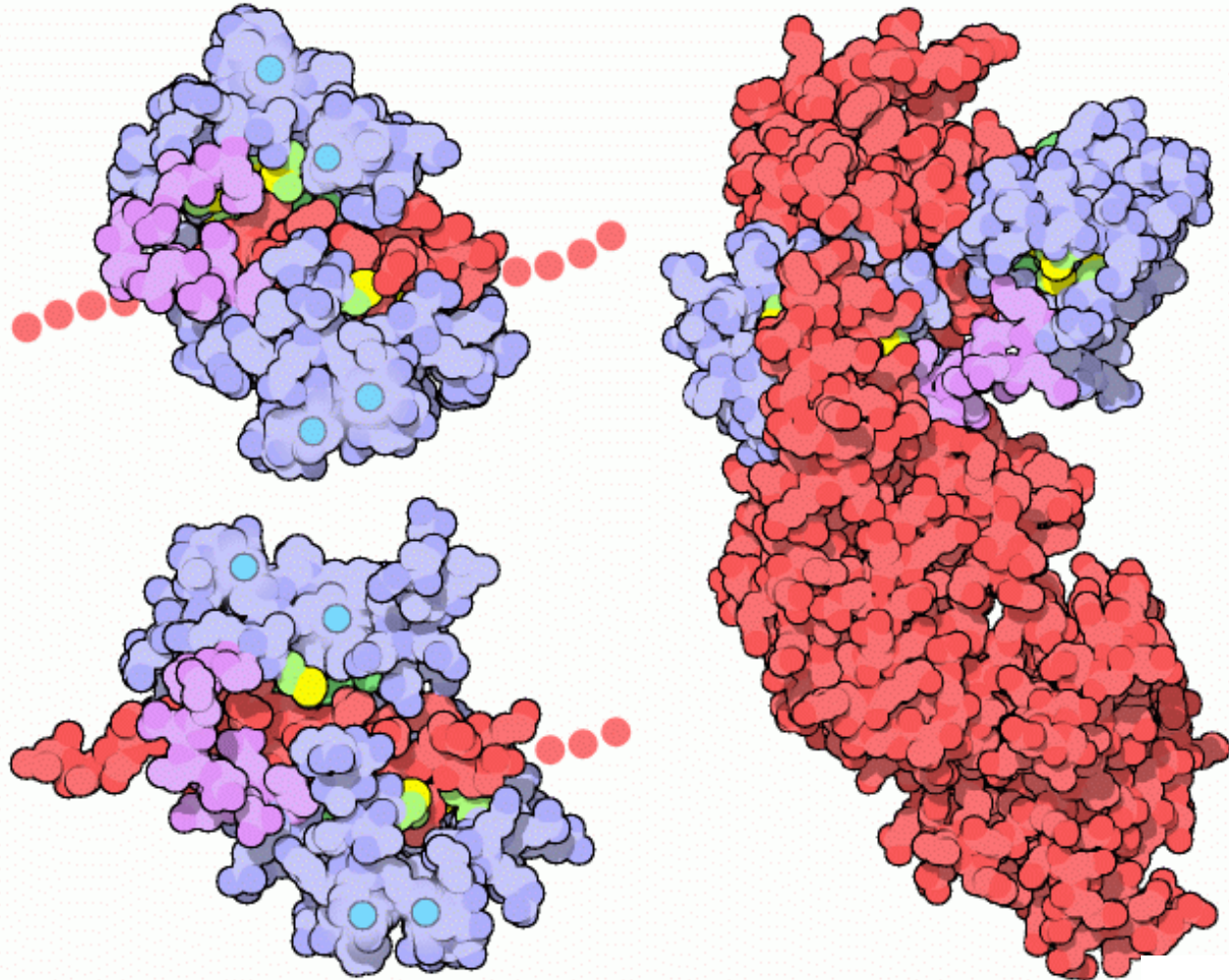
Calmodulin was PDB Molecule of the Month for August 2003

Calmodulin is a molecular switch:

- If no calcium
 - Then keep sticky spots closed
- Else, calcium binds
 - Then open up the sticky spots

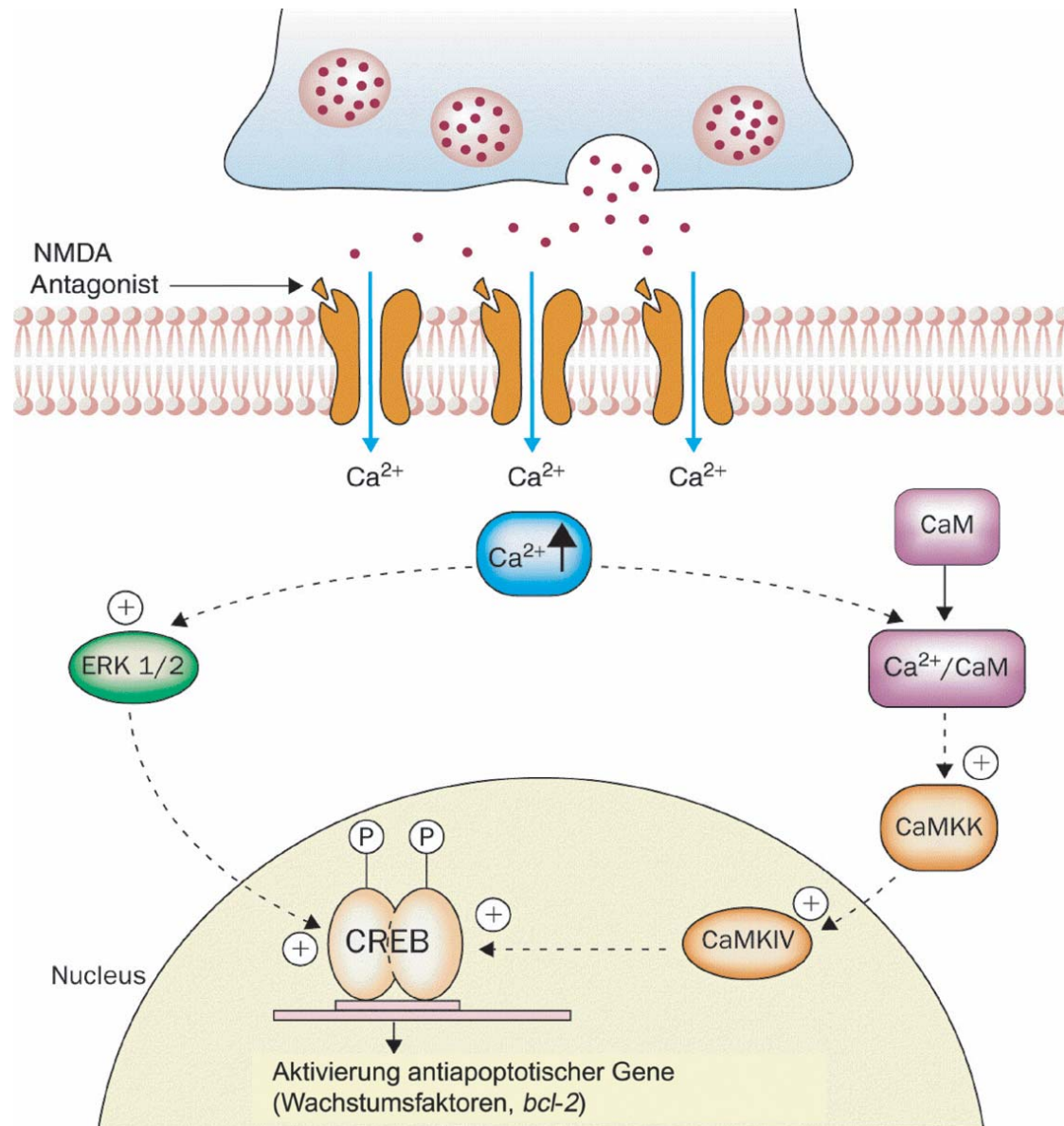


An Example: Calcium-Induced Structural Change in Calmodulin





One Role of CaM at the Synapse



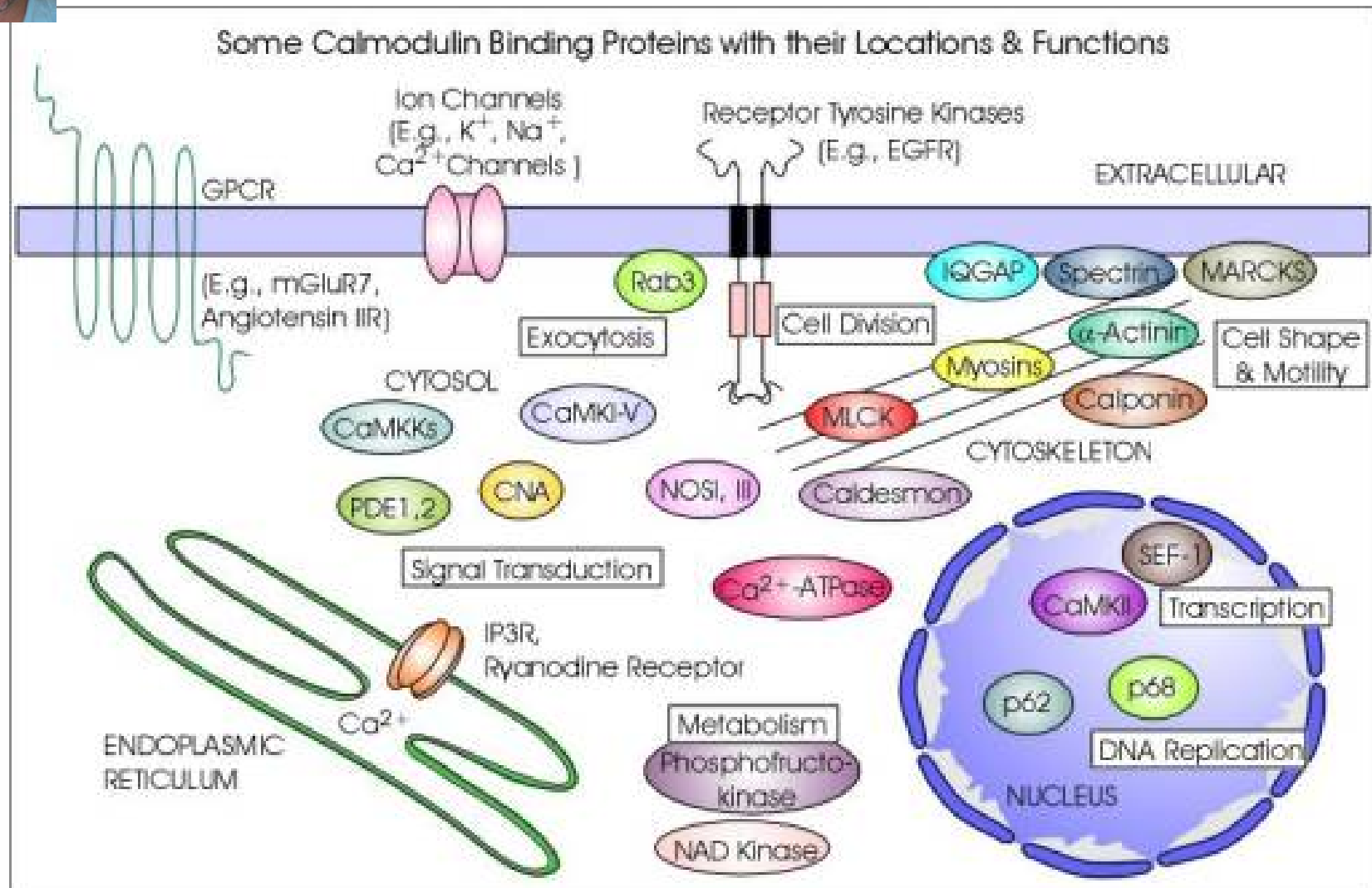


How many
calmodulin
binding proteins
can you name?
Stamp your
answer:

More than 20	More than 5
At least 1	zzzzzz



Some of the CaM Targets in the Cell





From Parts Lists to Systems-Level Understanding

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Two tasks:

1. System identification
2. Behavior analysis

How do the parts go together to make the functional system?



Additional Collections for Major Systems Biology Resources on the Web and Standards Movements in Systems Biology ...

Go to the NSDL K-12 page
resource list for this seminar

http://nsdl.org/resources_for/k12_teachers



<http://nsdl.org>





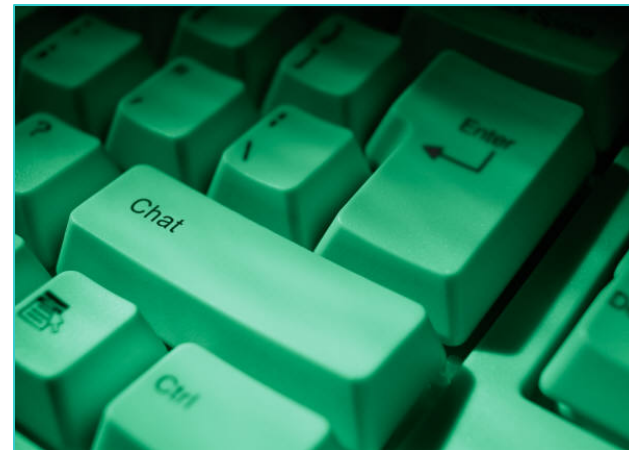
Which of the following is not one of the “Big 3” cellular networks?

Cell division	metabolic
signaling	gene-regulatory



How should we prepare students to contribute to, or at least understand post-genomic biology?

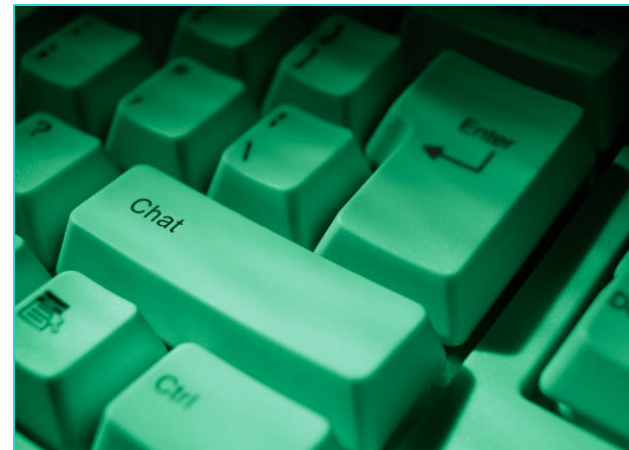
Write your ideas
on the chat





Have any of you mentioned systems biology in class? If so, what activities or lessons did you conduct on the topic?

Write your responses on the chat

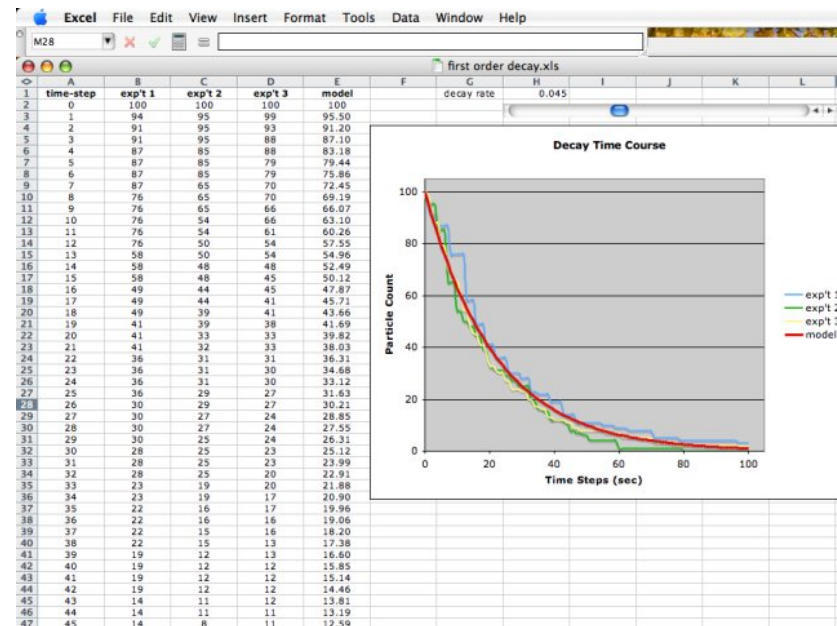




Under Development at Shodor: Dynamic Modeling Workbench

<http://www.shodor.org/~jeffk/dynModWB.html> (temporary site)

- **Analyze** time-course data from a virtual experiment
- **Diagram** the system using data
- **Build** a system diagram (Vensim model)
- **Run** the simulation
- **Compare** results to time-course data

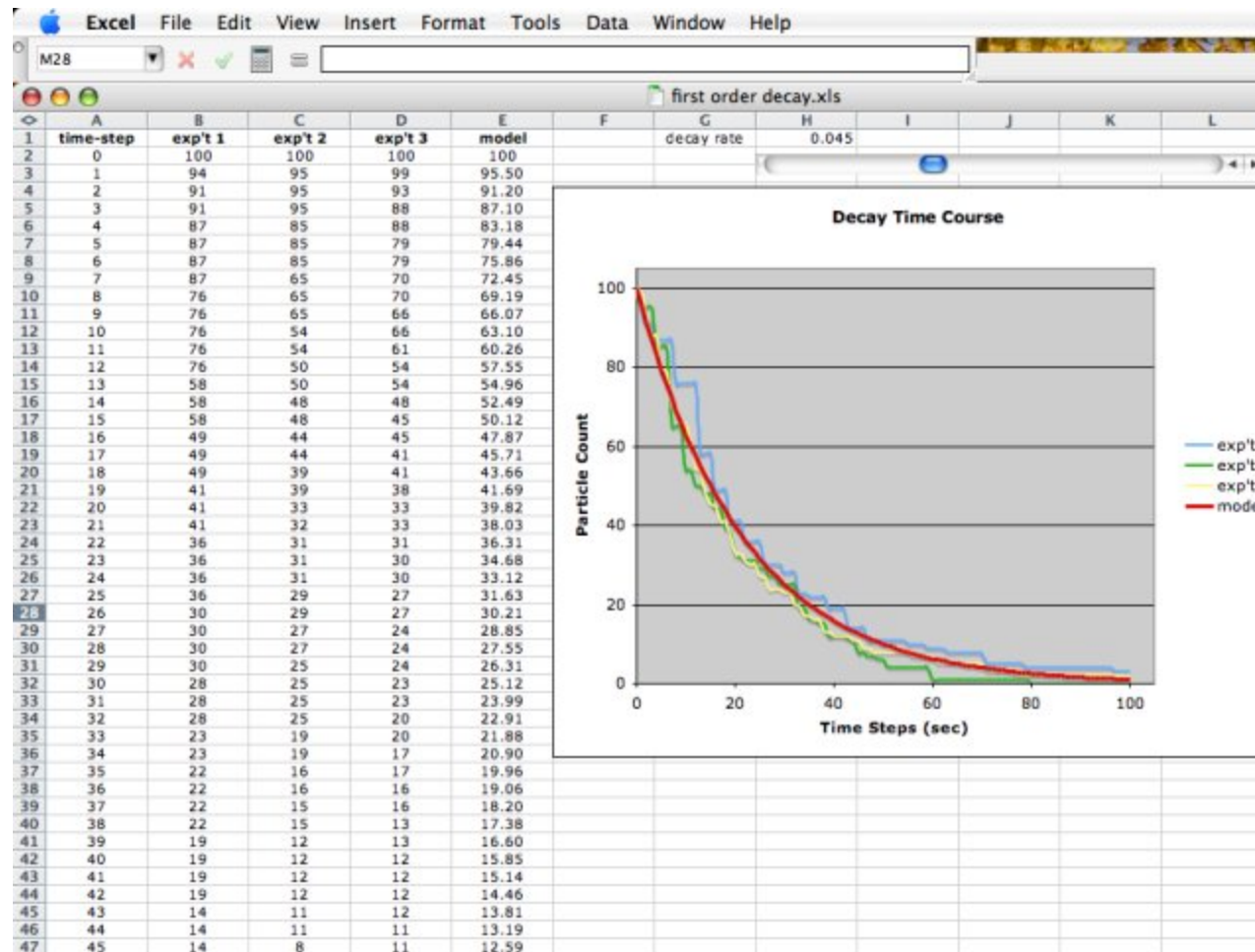


<http://nsdl.org>



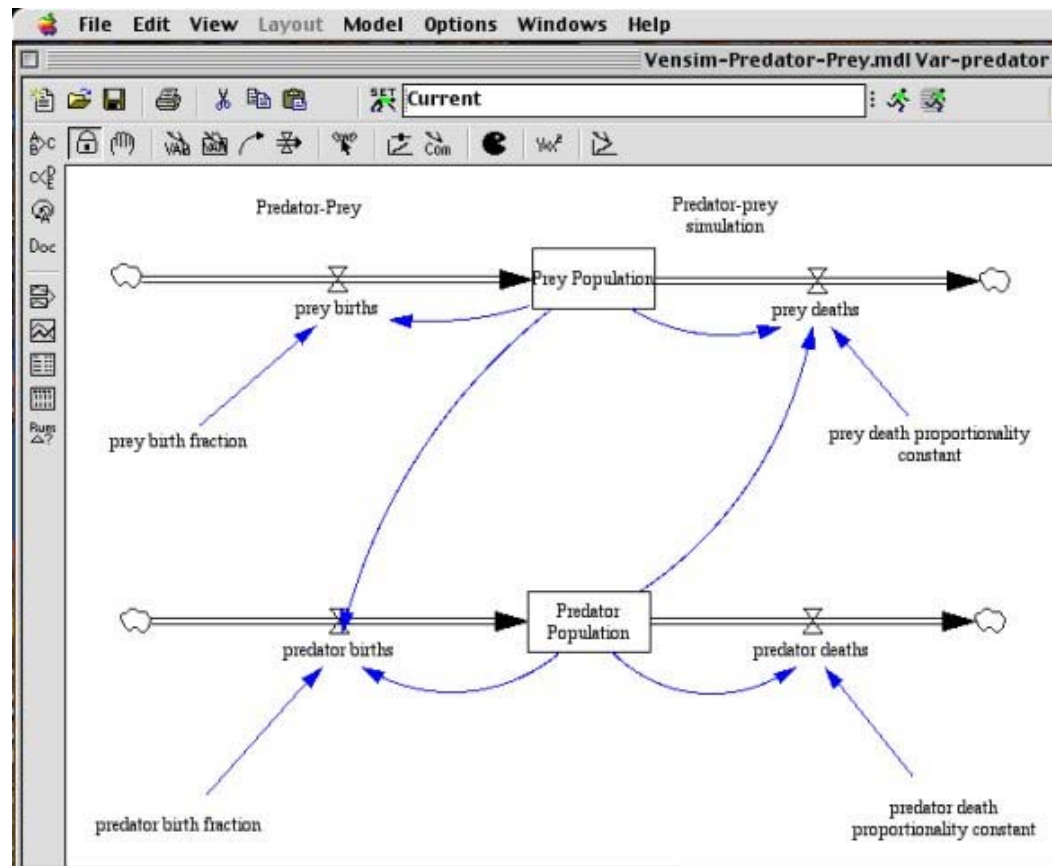


Step 1: Analyze Time-Course Data from a Virtual Experiment in Excel



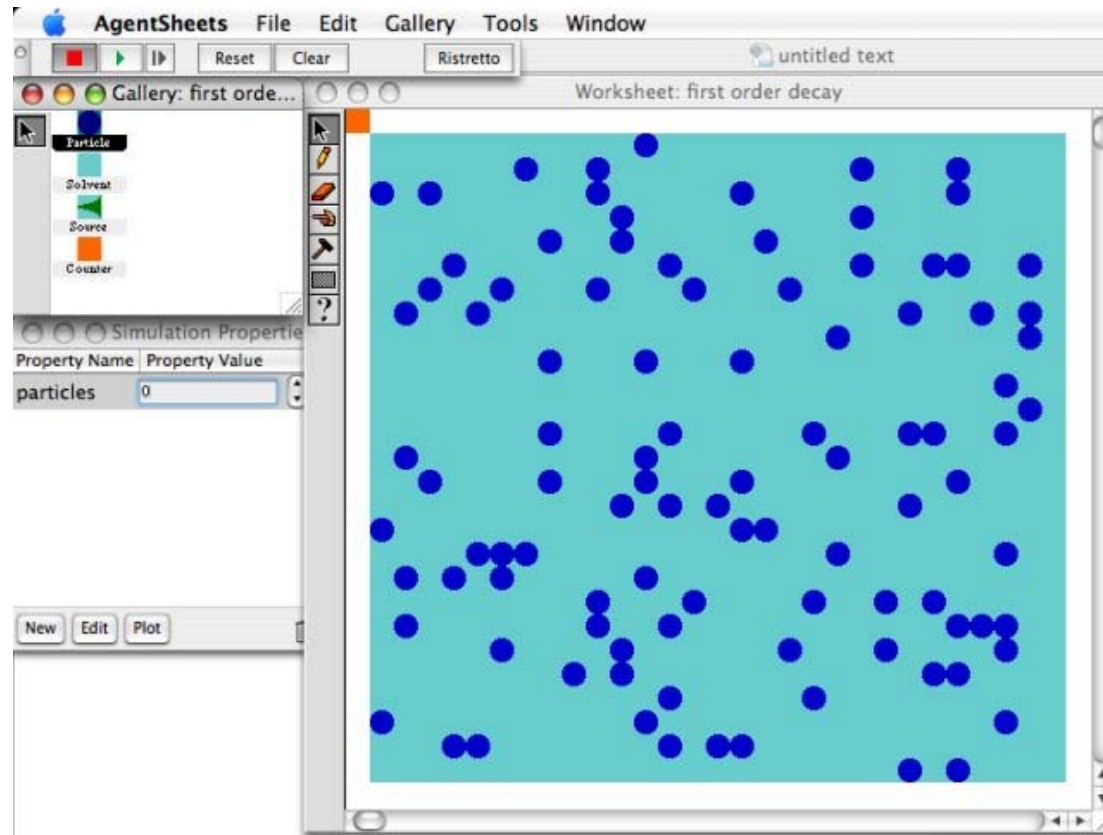


Step 2: Diagram the System, and Create and Run a Vensim Model



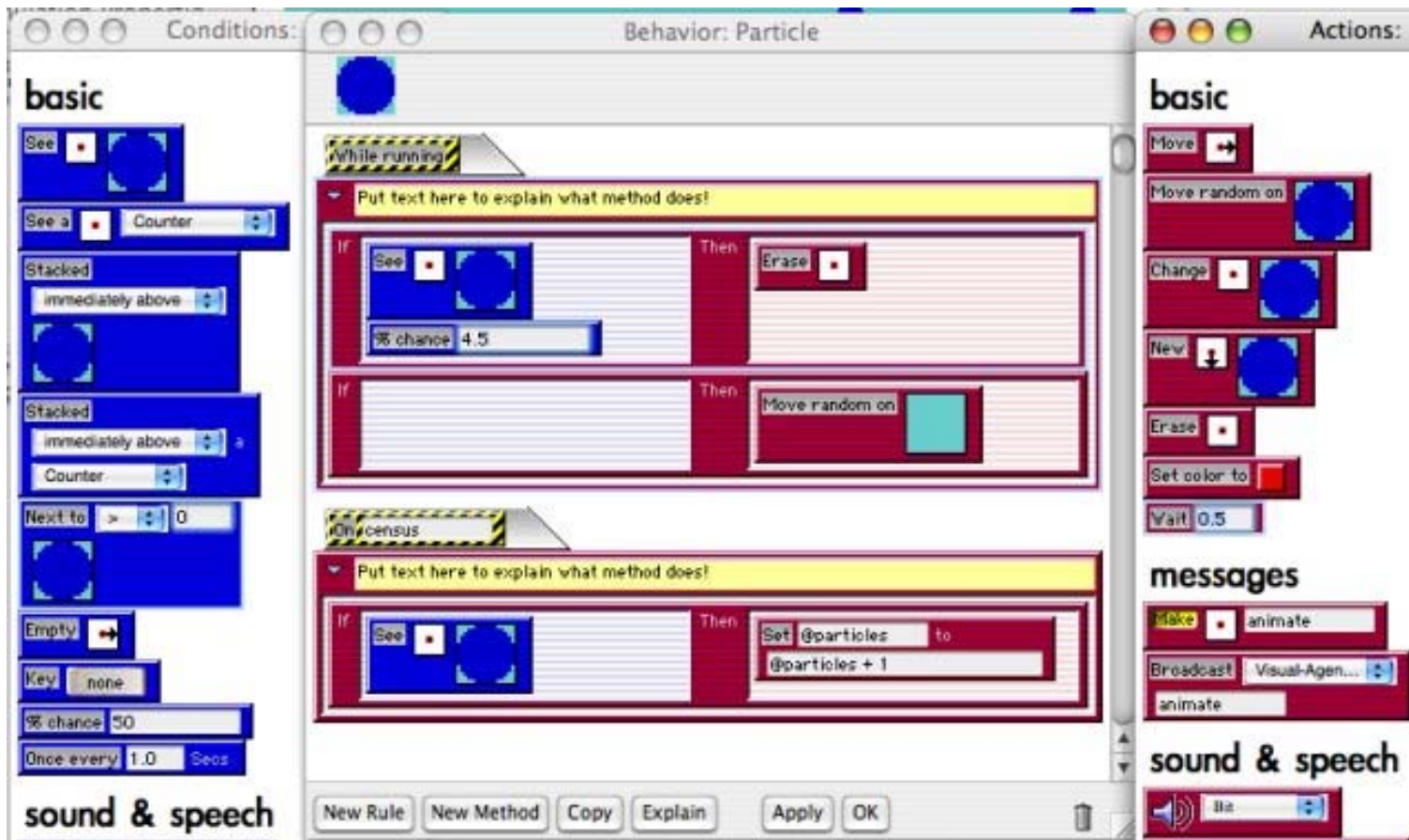


Step 3: Explore and modify the original Agent-Based Model that was used to produce the data





Agent Sheets allows model building with a graphical interface, but...





Shodor is always looking to work with passionate educators!



Dr. Jeff Krause
jeff.krause@shodor.org

**THANK
YOU!**

<http://www.shodor.org>

<http://www.cserd.nsdli.org>



Go to <http://nsdl.org> and click on the K-12 audience page to:

- Download our Seminar Resource List
- Utilize our blog featuring our presenters for the Fall Series sharing their insights on careers in science and science education:
<http://expertvoices.nsdl.org/2007fall-nsta-sems/>



<http://nsdl.org>





<http://www.lluminate.com>

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Welcome to The NSTA Learning Center

Get the Help, When You Need It

NSTA developed the Learning Center as a professional development website to help address your classroom needs and busy schedule. Using this site, you can gain access to more than 1,200 different resources and opportunities, such as:

- Over [1,000 NSTA Journal articles](#) (230 of them available FREE of charge)—many containing high-quality lesson plans.
- More than [35 FREE Science Objects](#) (one- to two-hour interactive simulation-based learning experiences).
- More than [125 e-chapters](#) from selected books and series (40 chapters FREE of charge).
- FREE weekly [live Web Seminars](#) where you can interact with experts from NASA, NOAA, FDA, NSF, and the NSDL Community.
- More than [20 SciGuides](#) (A resource to help teachers integrate the internet into the classroom).



PLUS: NSTA has also developed a suite of practical tools called [My Library](#), [My Notepad](#), and [My Transcript](#). Use these tools to organize, personalize, and document your professional growth within the Learning Center.

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National Science Teachers Association

Gerry Wheeler, Executive Director

Frank Owens, Associate Executive Director
Conferences and Programs

Al Byers, Assistant Executive Director e-Learning

NSTA Web Seminars

Flavio Mendez, Director

Danielle Troiano, Project Coordinator

Jeff Layman, Technical Coordinator





- *NASA: Successful Strategies for Involving Parents in Education*

December 12, 2007

- *IPY: The Role of Polar Regions in Earth's Changing Climate System*

December 13, 2007

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