Models By Examples

Simulating Light

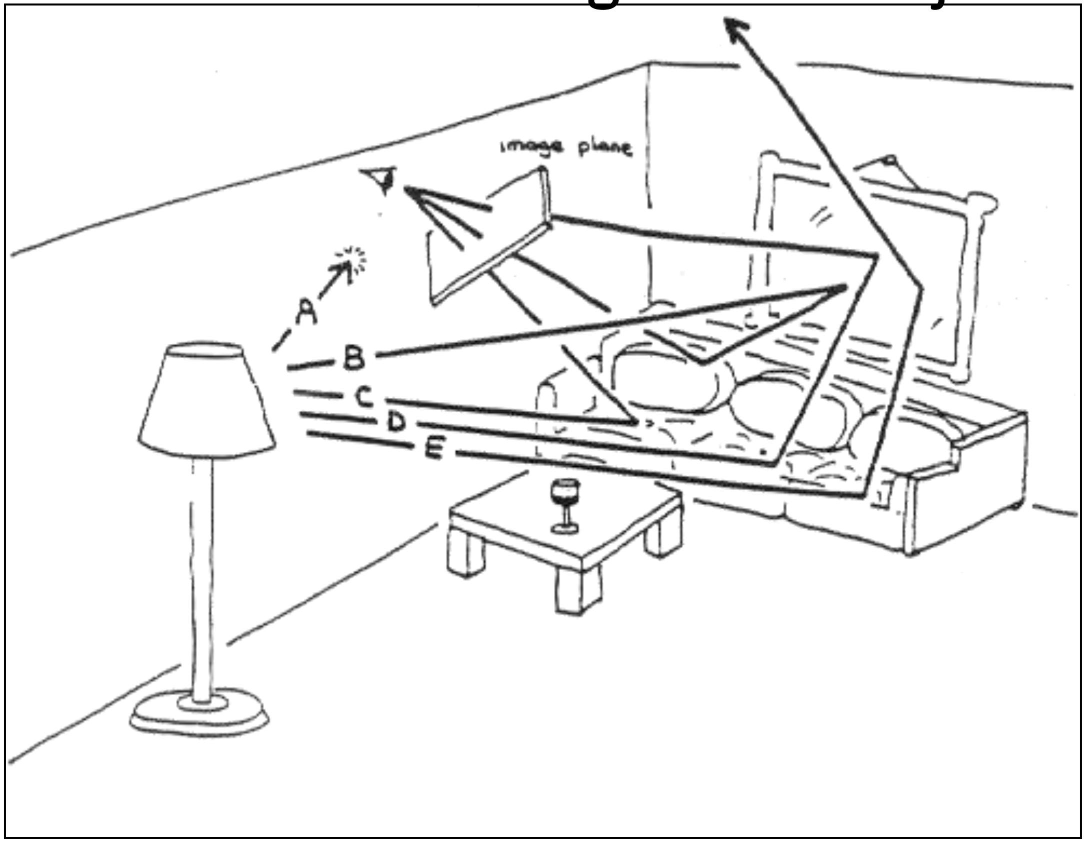
Illumination model

Used to simulate the interaction of light with objects

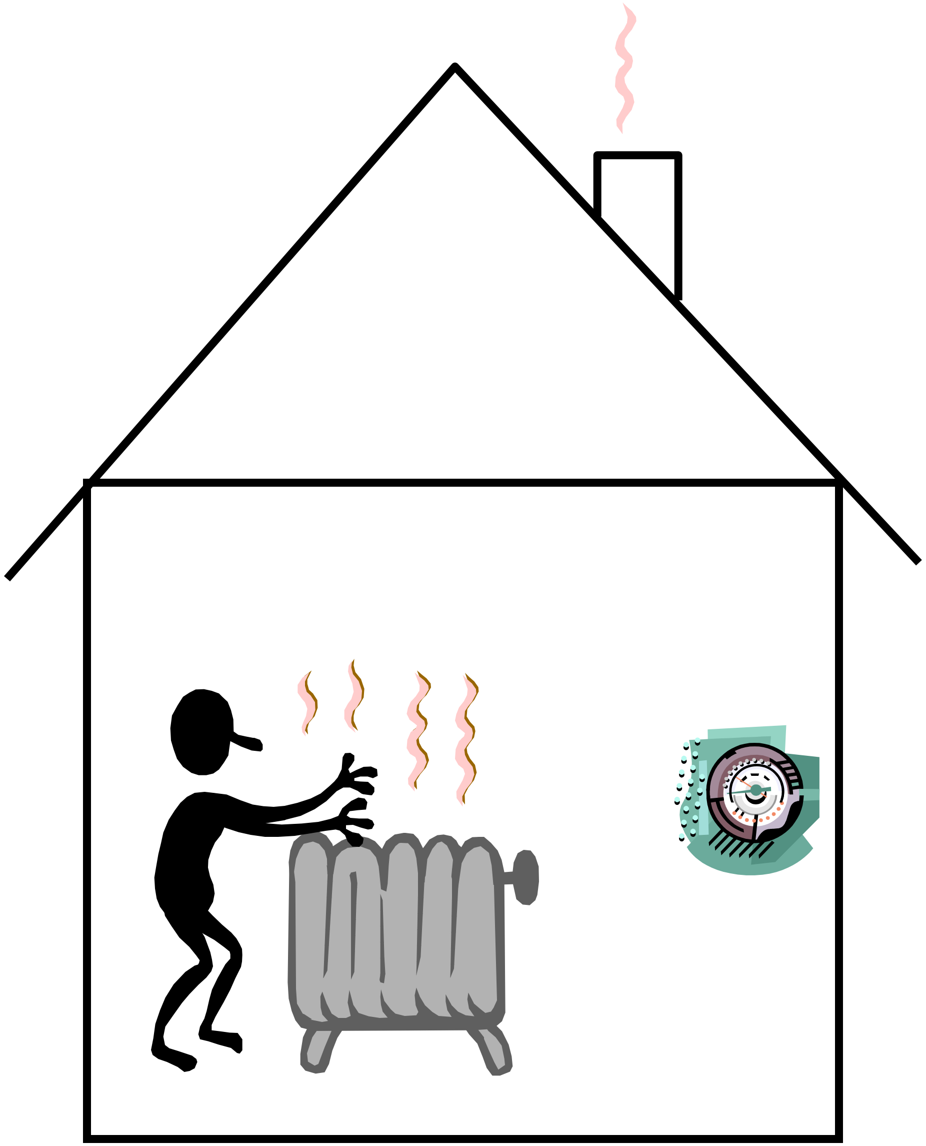
Objects are

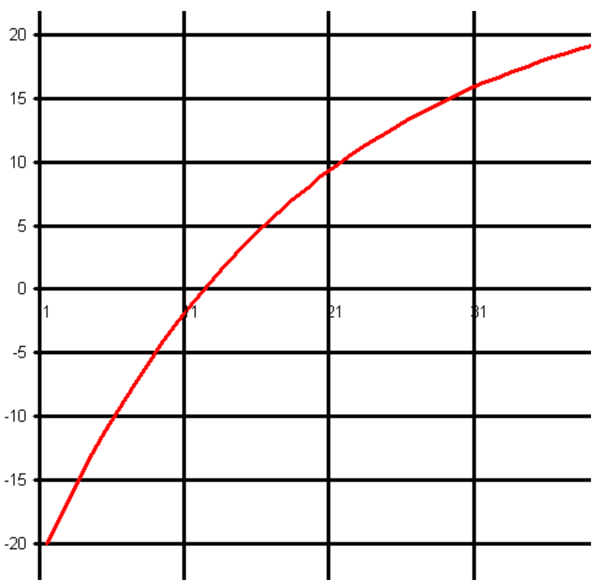
Shaded

Rendered

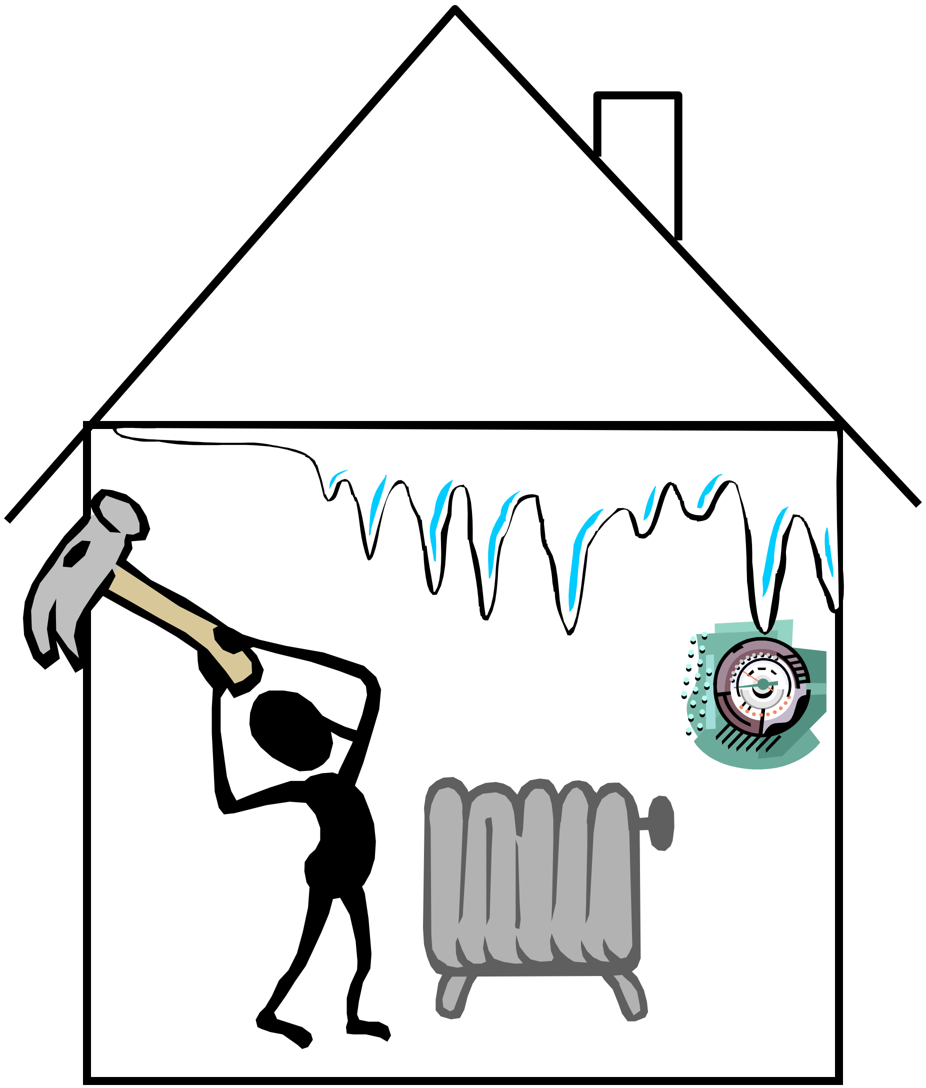


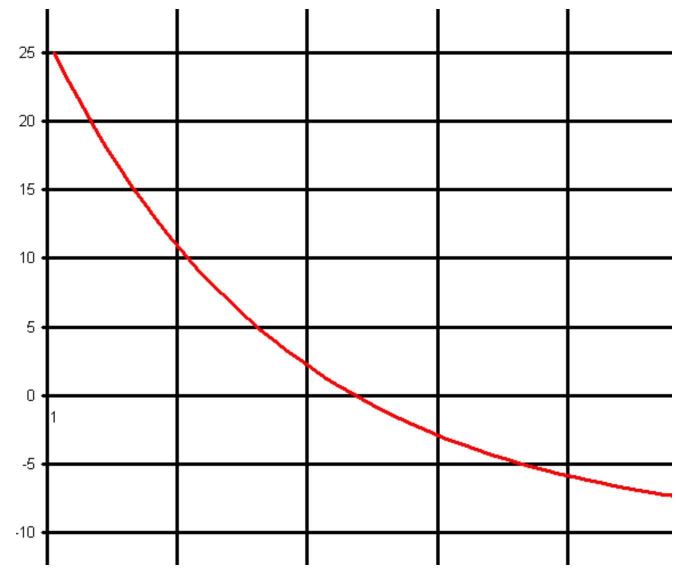
Continuous Model: Heating





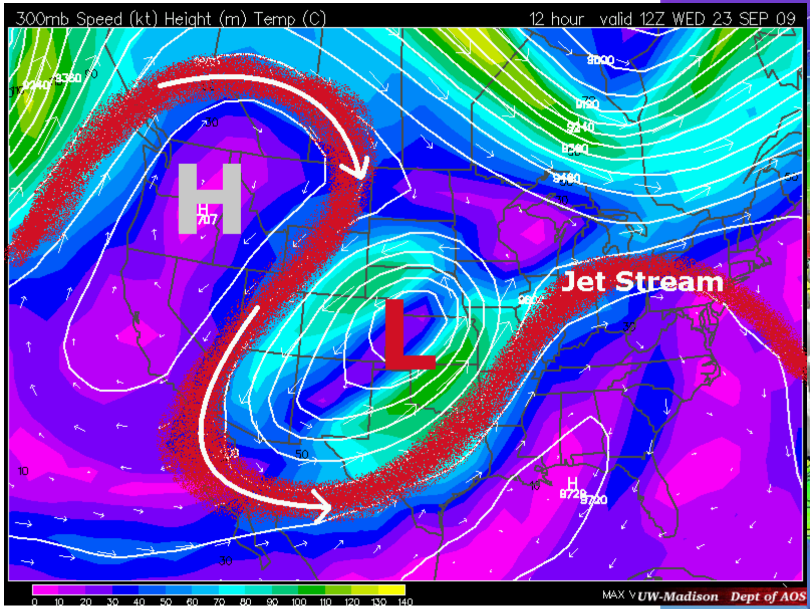
Continuous Model: Cooling

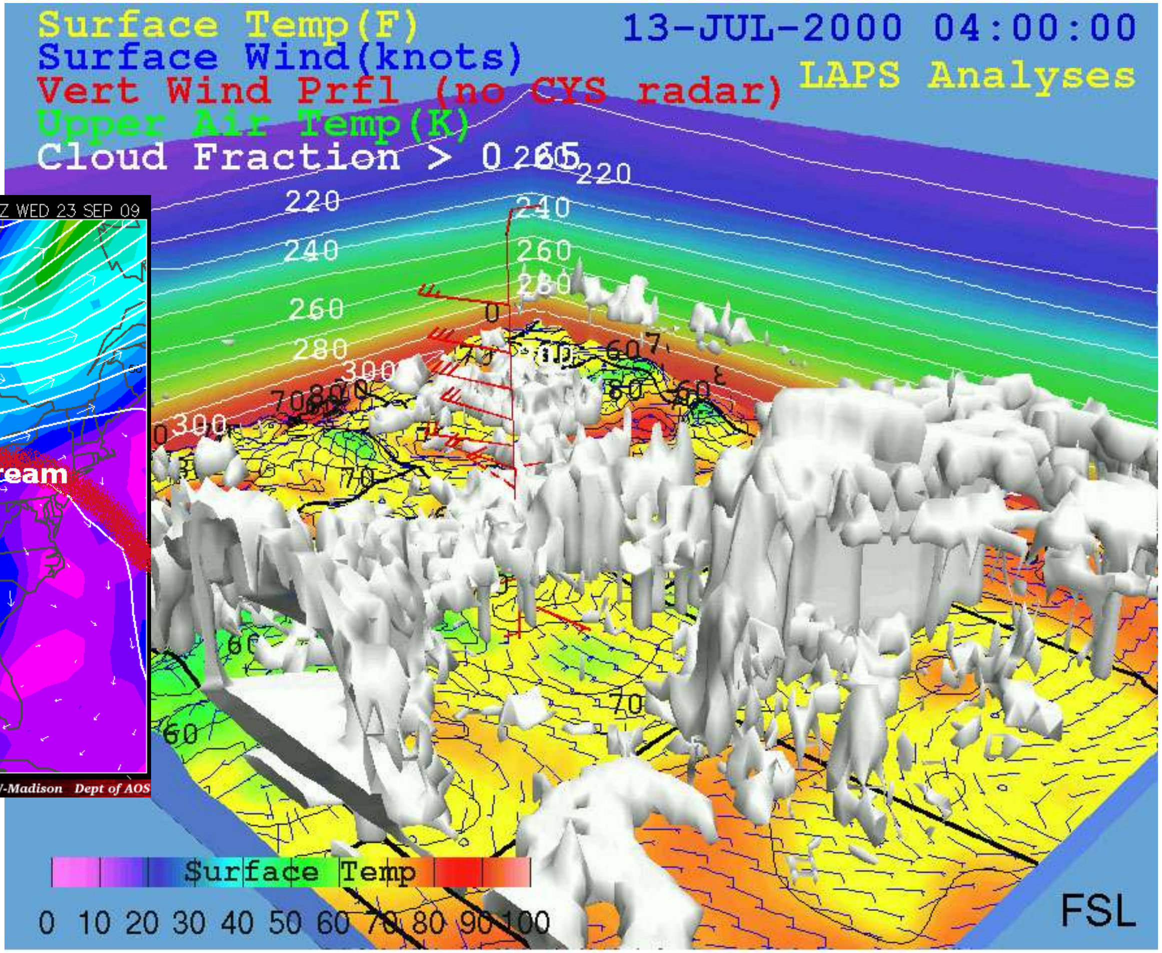




Meteorological Models

Weather – A Continuous Model

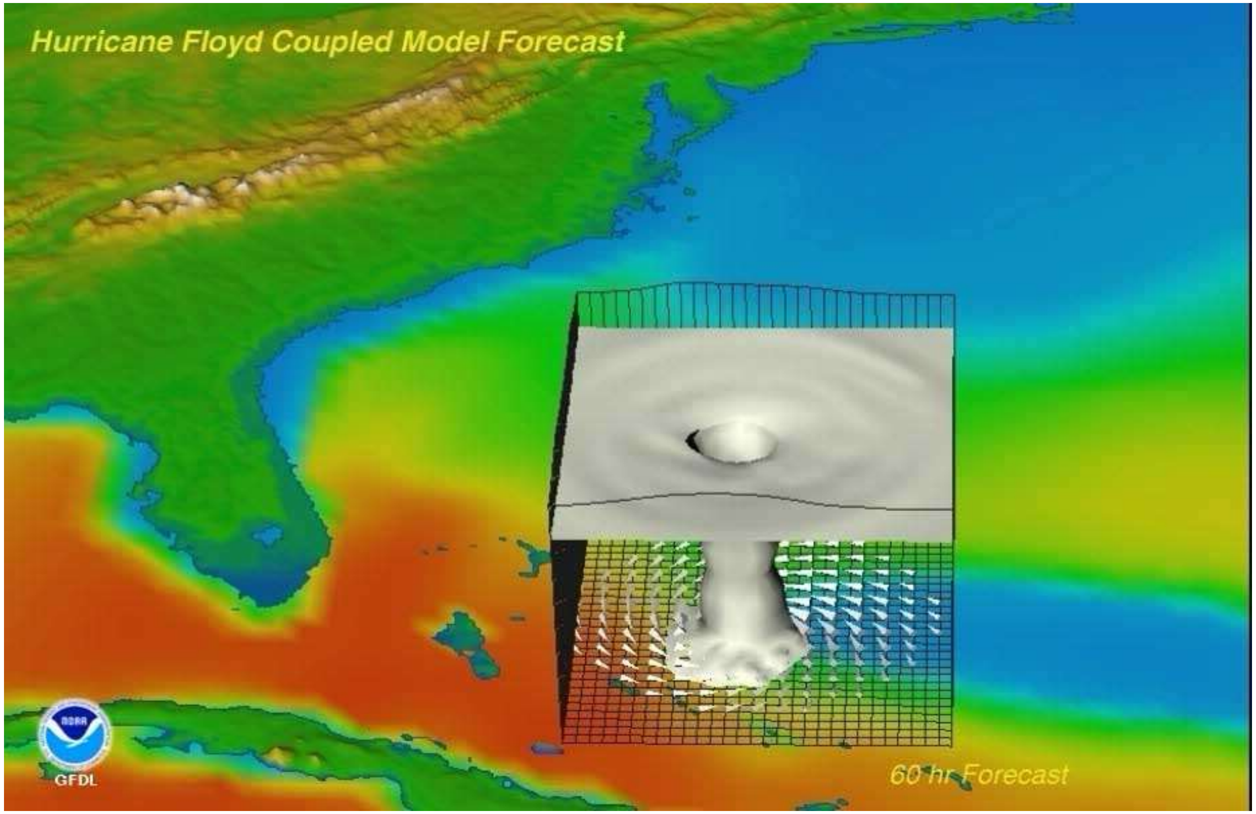




- LAPS Analysis for Colorado
- From Southeast
- Wind Profile Every 50 mb
- Highest is 100mb
- Surface Temp/Winds
- Upper Air Temp
- Cloud Fraction

Hurricanes – A Continuous Model

$$\frac{1}{2}\rho v^2 + \rho g z + p = q + \rho g h = p_0 + \rho g z = \text{constant}$$



Meteorological Models

Horizontal momentum:

$$\frac{\partial p^* u}{\partial t} = -m^2\left[\frac{\partial p^* uu/m}{\partial x} + \frac{\partial p^* vu/m}{\partial y}\right] - \frac{\partial p^* u\sigma}{\partial \sigma} + uDIV$$
$$-\frac{mp^*}{\rho}\left[\frac{\partial p'}{\partial x} - \frac{\sigma}{p^*}\frac{\partial p^*}{\partial x}\frac{\partial p'}{\partial \sigma}\right] - p^* fv + D_u$$
$$\frac{\partial p^* v}{\partial t} = -m^2\left[\frac{\partial p^* uv/m}{\partial x} + \frac{\partial p^* vv/m}{\partial y}\right] - \frac{\partial p^* v\sigma}{\partial \sigma} + vDIV$$
$$-\frac{mp^*}{\rho}\left[\frac{\partial p'}{\partial y} - \frac{\sigma}{p^*}\frac{\partial p^*}{\partial y}\frac{\partial p'}{\partial \sigma}\right] - p^* fu + D_v$$

Vertical momentum:

$$\frac{\partial p^* w}{\partial t} = -m^2\left[\frac{\partial p^* uv/m}{\partial x} + \frac{\partial p^* vw/m}{\partial y}\right] - \frac{\partial p^* w\sigma}{\partial \sigma} + wDIV$$
$$+p^* g\frac{p_0}{\rho}\left[\frac{1}{p^*}\frac{\partial p'}{\partial \sigma} + \frac{T_v'}{T} - \frac{T_0 p'}{T p_0}\right] - p^* g\left[(q_c + q_r)\right] + D_w$$

Pressure:

$$\frac{\partial p^* p'}{\partial t} = -m^2\left[\frac{\partial p^* up'/m}{\partial x} + \frac{\partial p^* vp'/m}{\partial y}\right] - \frac{\partial p^* p'\sigma}{\partial \sigma} + p'DIV$$
$$-m^2 p^* \gamma p\left[\frac{\partial u/m}{\partial x} - \frac{\sigma}{mp^*}\frac{\partial p^*}{\partial x}\frac{\partial u}{\partial \sigma} + \frac{\partial v/m}{\partial y} - \frac{\sigma}{mp^*}\frac{\partial p^*}{\partial y}\frac{\partial v}{\partial \sigma}\right]$$
$$+p_0 g\gamma p\frac{\partial w}{\partial \sigma} + p^* p_0 gw$$

Temperature:

$$\frac{\partial p^* T}{\partial t} = -m^2\left[\frac{\partial p^* uT/m}{\partial x} + \frac{\partial p^* vT/m}{\partial y}\right] - \frac{\partial p^* T\sigma}{\partial \sigma} + T\,DIV$$
$$+\frac{1}{\rho c_p}\left[p^*\frac{Dp'}{Dt} - p_0 g p^* w - D_{p'}\right] + p^*\frac{Q}{c_p} + D_T,$$

where

$$DIV = m^2\left[\frac{\partial p^* u/m}{\partial x} + \frac{\partial p^* v/m}{\partial y}\right] + \frac{\partial p^* \sigma}{\partial \sigma},$$

and

$$\sigma = -\frac{p_0 g}{p^*}w - \frac{m\sigma}{p^*}\frac{\partial p^*}{\partial x}u - \frac{m\sigma}{p^*}\frac{\partial p^*}{\partial y}v.$$

How much math does it take to be a meteorologist?

Computational Biology

Computational Biology

The application of computer science to problems in biology

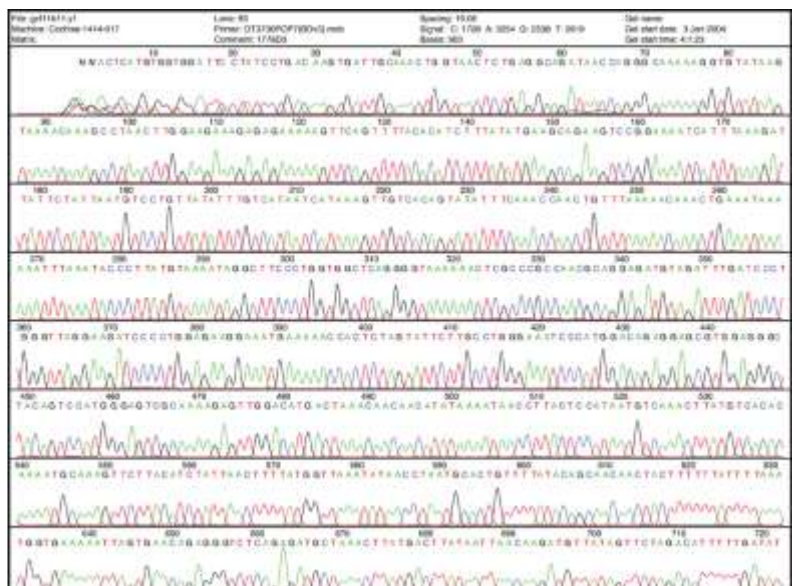
(or is it the other way around?? ☺)

Encompasses:

- bioinformatics
- computational biomodeling
- molecular modeling
- protein structure prediction

Computational Biology

- **Bioinformatics**
- Discovering and Processing DNA sequences
- Human Genome Project and Others

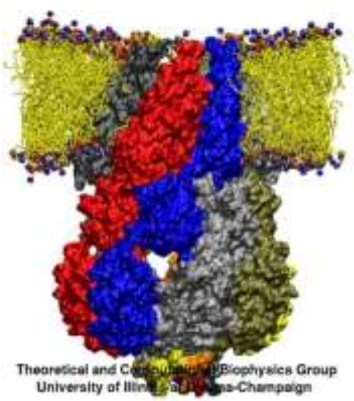


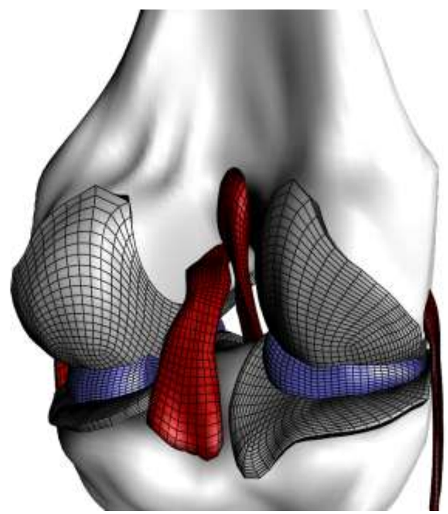
Computational Biology

- ## Computational Biomodeling
- The simulation of biological systems

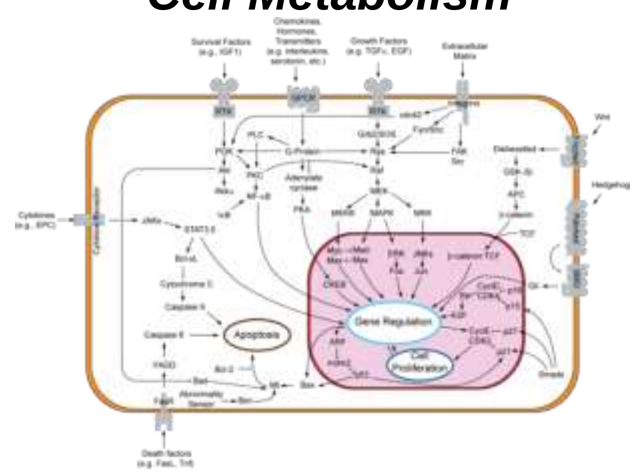
Knees

Cell Wall Protein



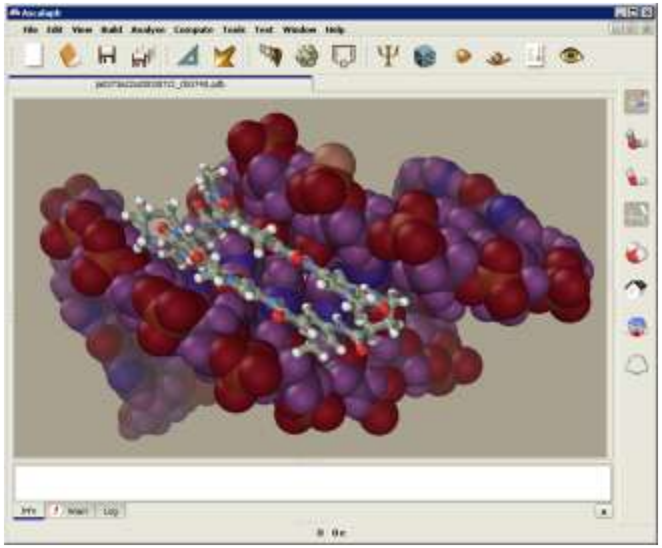


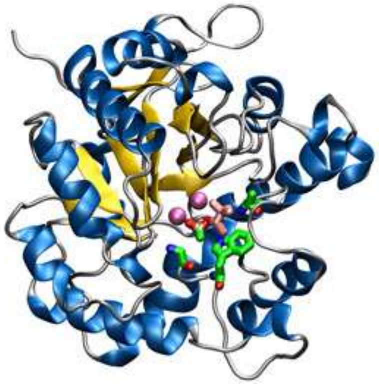
Cell Metabolism



Computational Biology

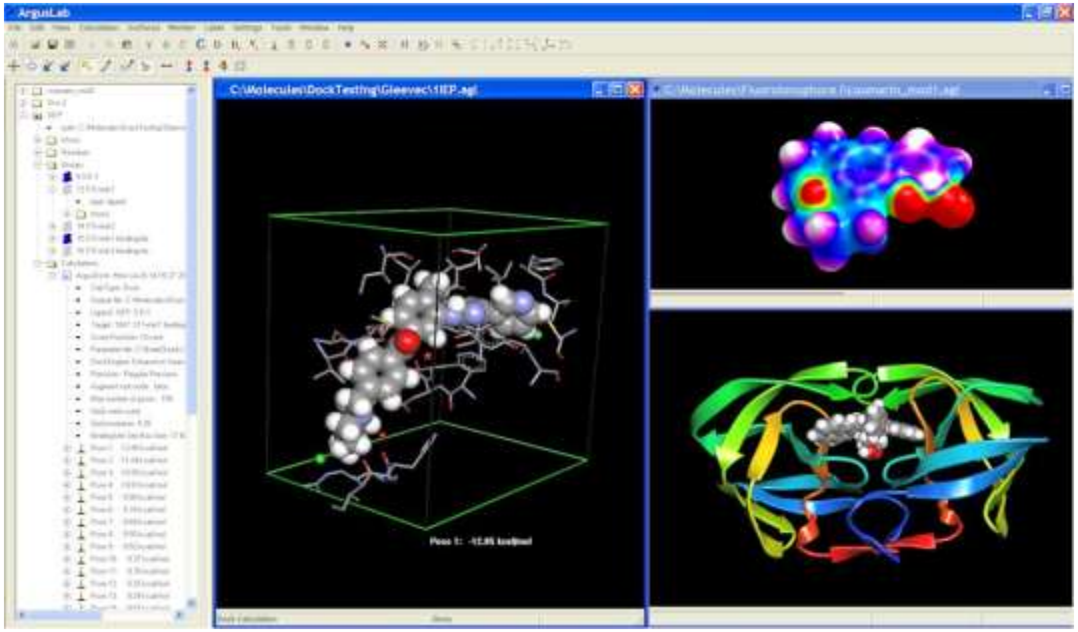
- **Protein Structure Modeling**
- Simulating 3-Dimensional Structure and Function of Protein Molecules





Computational Biology

- **Molecular Modeling**
- Simulating Structure and Function of Chemical Molecules (usually drug discovery)



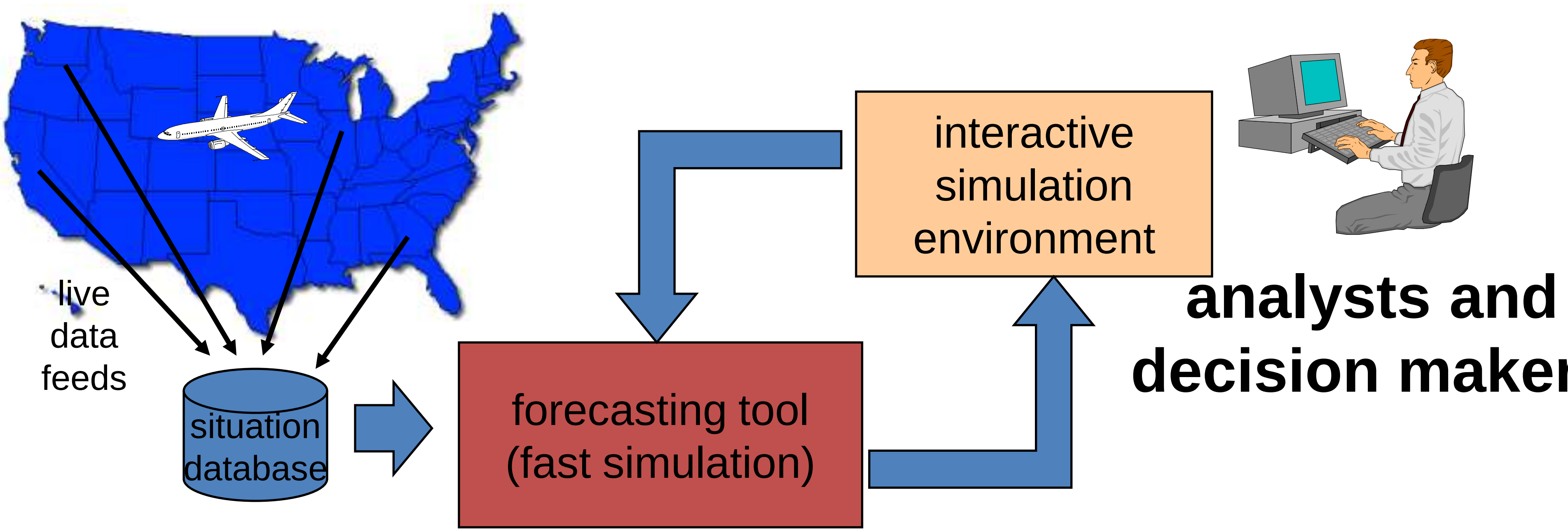
Applications: System Analysis

"Classical" application of simulation

- Telecommunication networks
- Transportation systems
- Electronic systems (e.g., microelectronics, computer systems)
- Battlefield simulations (blue army vs. red army)
- Ecological systems
- Manufacturing systems
- Logistics

Focus typically on planning, system design

Applications: On-Line Decision Aids



Simulation tool is used for fast analysis of alternate courses of action in time critical situations

- Initialize simulation from situation database
- Faster-than-real-time execution to evaluate effect of decisions

Applications: air traffic control, battle management

Simulation results may be needed in only seconds

Discrete-Time Models

Lecture 1

When To Use Discrete-Time Models

Discrete models or ***difference equations*** are used to describe biological phenomena or events for which it is natural to regard time at fixed (discrete) intervals.

Examples:

- The size of an insect population in year *i*;
- The proportion of individuals in a population carrying a particular gene in the *i*-th generation;
- The number of cells in a bacterial culture on day *i*;
- The concentration of a toxic gas in the lung after the *i*-th breath;
- The concentration of drug in the blood after the *i*-th dose.

What does a model for such situations look like?

- Let x_n be the quantity of interest after n time steps.
- The model will be a rule, or set of rules, describing how x_n changes as time progresses.
- In particular, the model describes how x_{n+1} depends on x_n (and perhaps x_{n-1}, x_{n-2}, …).

- In general: $x_{n+1} = f(x_n, x_{n-1}, x_{n-2}, \ldots)$

- For now, we will restrict our attention to:

$$x_{n+1} = f(x_n)$$

Terminology

The relation $x_{n+1} = f(x_n)$ is a difference equation; also called a recursion relation or a map.

Given a difference equation and an initial condition, we can calculate the iterates x_1, x_2 ..., as follows:

$$x_1 = f(x_0)$$

$$x_2 = f(x_1)$$

$$x_3 = f(x_2)$$

$$\vdots$$

The sequence $\{x_0, x_1, x_2, \ldots\}$ is called an orbit.

Question

- Given the difference equation $x_{n+1} = f(x_n)$ can we make predictions about the characteristics of its orbits?

Modeling Paradigm

- Future Value = Present Value + Change

  $$x_{n+1} = x_n + \Delta x_n$$

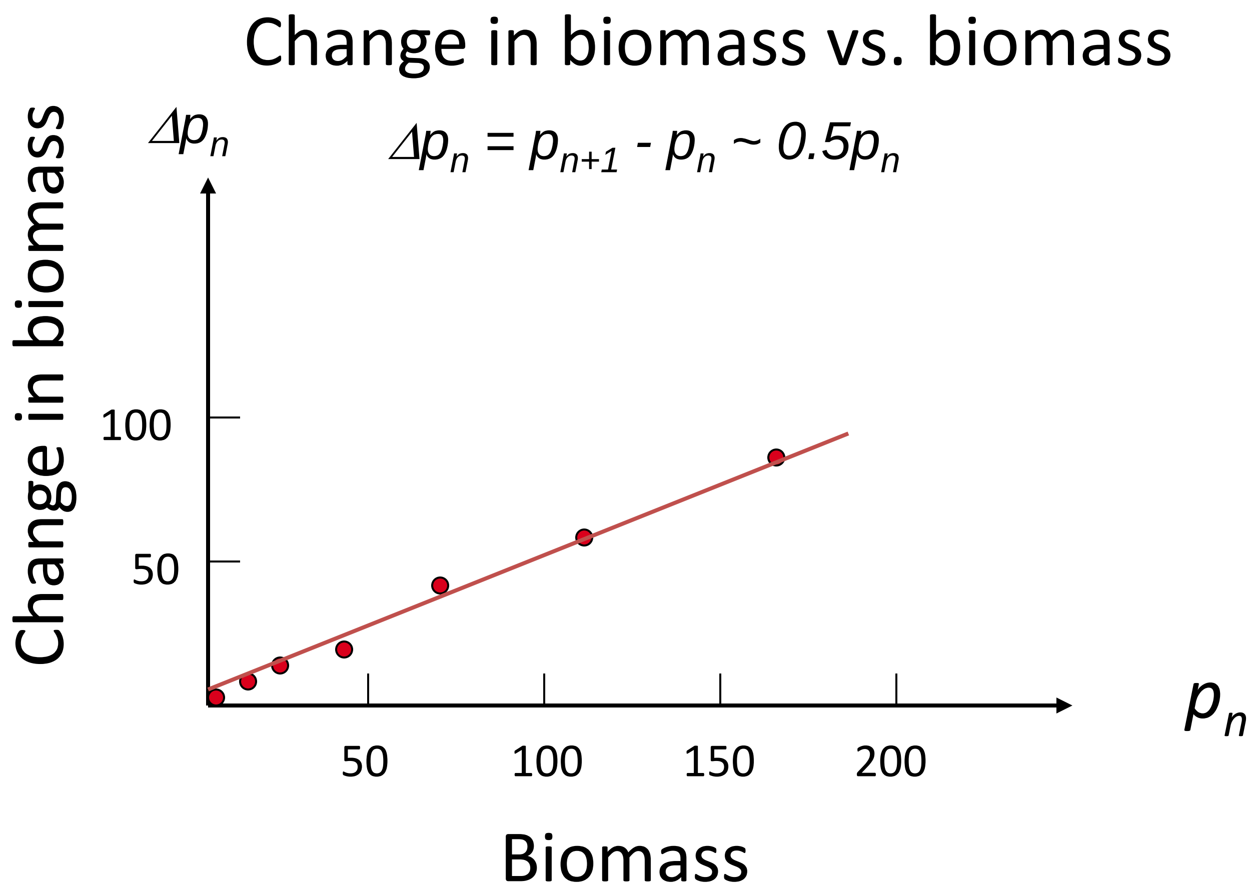
- Goal of the modeling process is to find a reasonable approximation for Δx_n that reproduces a given set of data or an observed phenomena.

Example: Growth of a Yeast Culture

The following data was collected from
an experiment measuring the growth of a yeast cultur

Time (hours)	Yeast biomass	Change in biomass
n	p_n	$\Delta p_n = p_{n+1} - \Delta p_n$
0	9.6	8.7
1	18.3	10.7
2	29.0	18.2
3	47.2	23.9
4	71.1	48.0
5	119.1	55.5
6	174.6	82.7
7	257.3	

Change in Population is Proportional to the Population



Explosive Growth

- From the graph, we can estimate that

  $\Delta p_n = p_{n+1} - p_n \sim 0.5p_n$ and we obtain the model

$$p_{n+1} = p_n + 0.5p_n = 1.5p_n$$

The solution is:

$$p_{n+1} = 1.5(1.5p_{n-1}) = 1.5[1.5(1.5p_{n-2})] = \ldots = (1.5)^{n+1} p_0$$

$$\Rightarrow \quad p_n = (1.5)^n p_0.$$

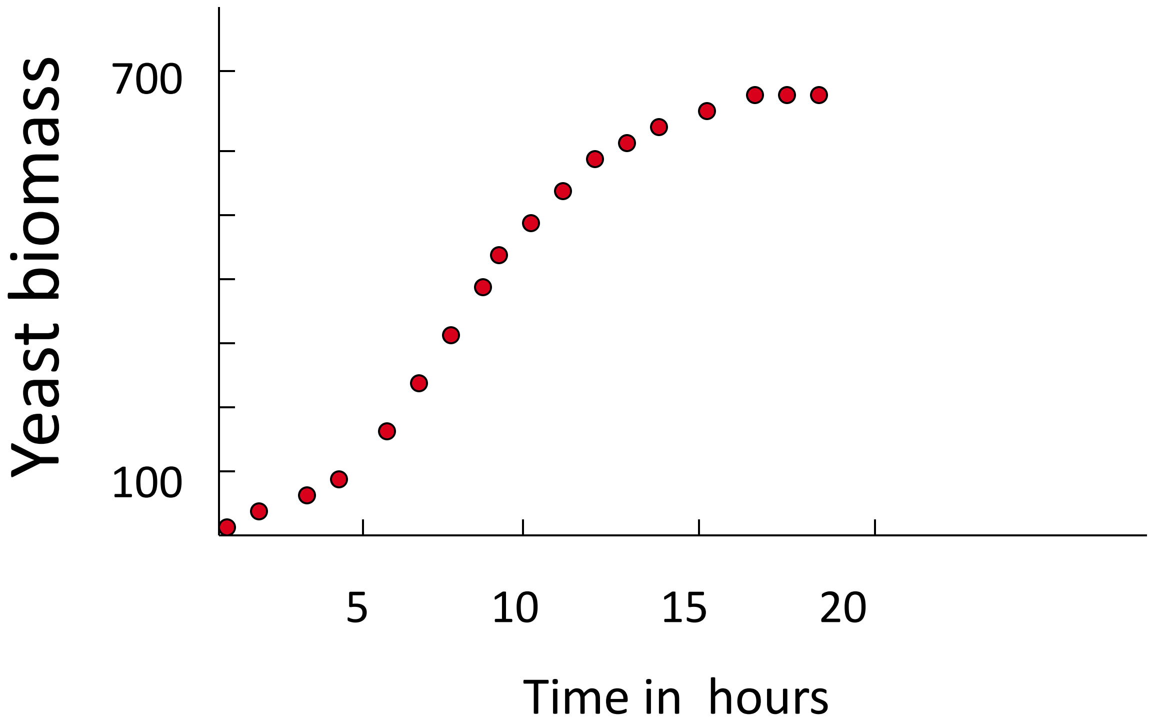
This model predicts a population that increases forever.

Clearly we should re-examine our data so that we can come up with a better model.

Example: Growth of a Yeast Culture Revisited

Time (hours) n	Yeast biomass p_n	Change in biomass $\Delta p_n = p_{n+1} - \Delta p_n$
0	9.6	8.7
1	18.3	10.7
2	29.0	18.2
3	47.2	23.9
4	71.1	48.0
5	119.1	55.5
6	174.6	82.7
7	257.3	93.4
8	350.7	90.3
9	441.0	72.3
10	513.3	46.4
11	559.7	35.1
12	594.8	34.6
13	629.4	11.5
14	640.8	10.3
15	651.1	4.8
16	655.9	3.7
17	659.6	2.2
18	661.8	

Yeast Biomass Approaches a Limiting Population Level



The limiting yeast biomass is approximately 665.

Refining Our Model

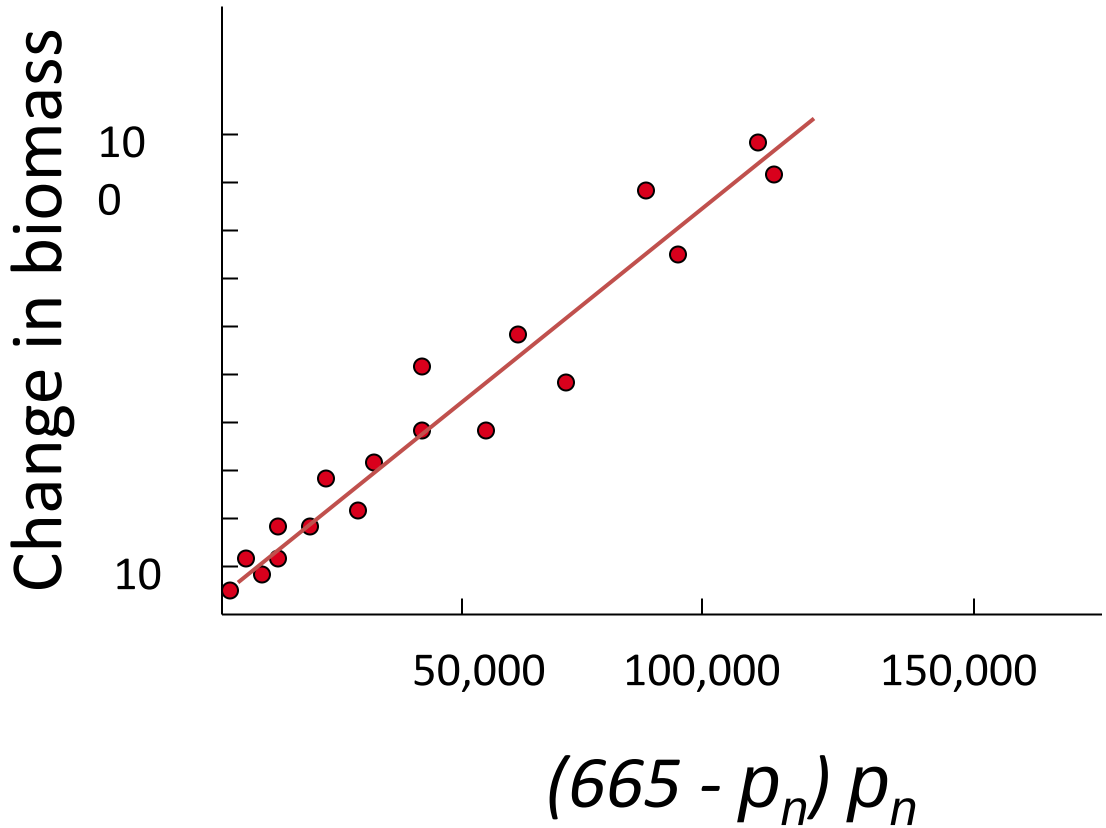
- Our original model: $\Delta p_n = 0.5p_n$
  $p_{n+1} = 1.5p_n$
- Observation from data set: The change in biomass becomes smaller as the resources become more constrained, in particular, as p_n approaches 665.

- Our new model: $\Delta p_n = k(665 - p_n)\, p_n$
  $p_{n+1} = p_n + k(665 - p_n)\, p_n$

Testing the Model

- We have hypothesized $\Delta p_n = k(665-p_n)\, p_n$ ie, the change in biomass is proportional to the product $(665-p_n)\, p_n$ with constant of proportionality k.
- Let's plot Δp_n *vs.* $(665-p_n)\, p_n$ to see if there is reasonable proportionality.
- If there is, we can use this plot to estimate k.

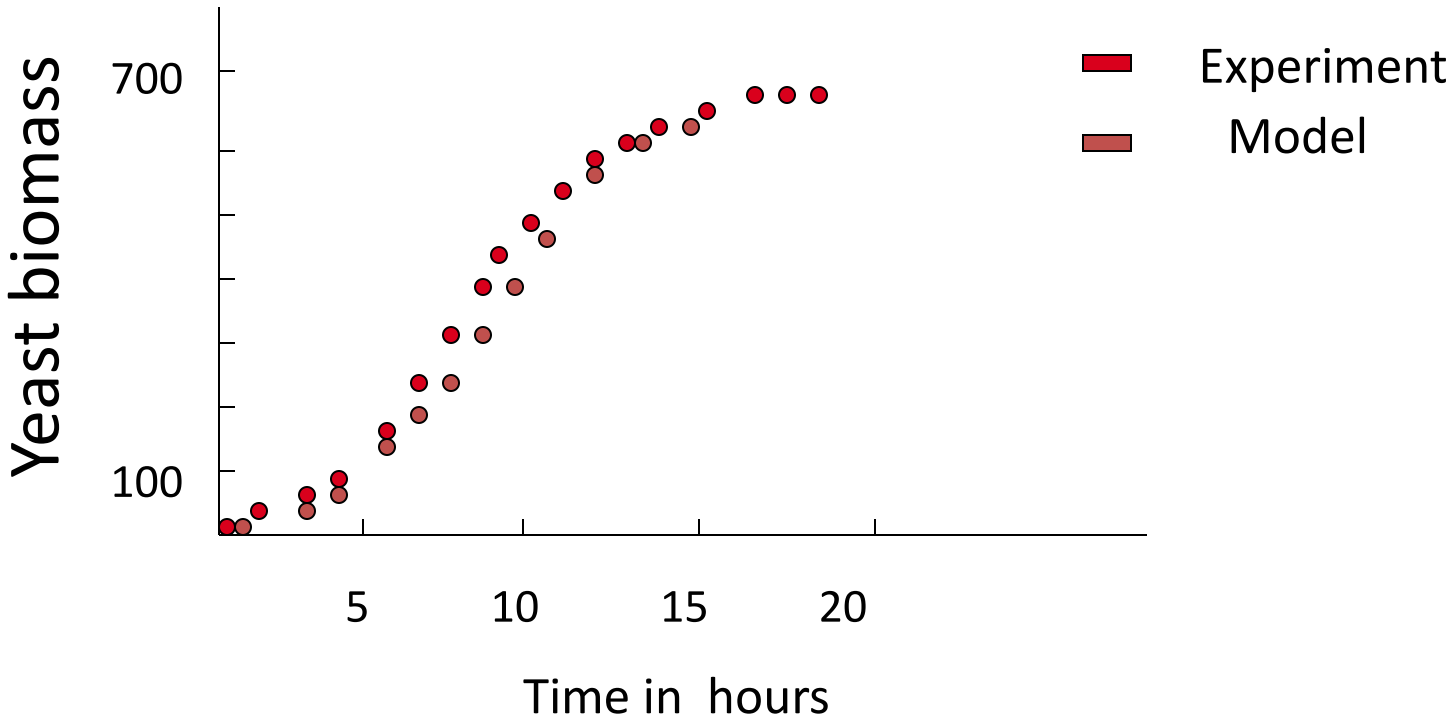
Testing the Model Continued



Our hypothesis seems reasonable, and the constant of Proportionality is $k \sim 0.00082$.

Comparing the Model to the Data

Our new model: $p_{n+1} = p_n + 0.00082(665\text{-}p_n)\ p_n$



The Discrete Logistic Model

$$x_{n+1} = x_n + k(N - x_n)\, x_n$$

- Interpretations
  - Growth of an insect population in an environment with limited resources
    - x_n = number of individuals after n time steps (e.g. years)
    - N = max number that the environment can sustain
  - Spread of infectious disease, like the flu, in a closed population
    - x_n = number of infectious individuals after n time steps (e.g. days)
    - N = population size

WHAT HAVE WE OBSERVED?

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \frac{1}{4!}x^4 + \frac{1}{5!}x^5 + \cdots$$

SERIES

$$\sin x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!} = x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 - \frac{1}{7!}x^7 + \cdots$$

$$\cos x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!} = 1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 - \frac{1}{6!}x^6 + \cdots$$

ARE OTHER FUNCTIONS SIMILAR?

PRINCIPLE

"EVERY" "REASONABLE" FUNCTION f IS OF THE FORM

$$f(x) = \sum_{k=0}^{\infty} c_k x^k = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + \cdots$$

FOR SOME $\{c_k\}$

SERIES

HOW TO COMPUTE THE c_k?

DEFINITION

THE TAYLOR SERIES OF $f(x)$ AT $x=0$ IS:

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k = f(0) + \left.\frac{df}{dx}\right|_0 x + \frac{1}{2!}\left.\frac{d^2f}{dx^2}\right|_0 x^2 + \frac{1}{3!}\left.\frac{d^3f}{dx^3}\right|_0 x^3 + \cdots$$

That is, $C_k = \frac{f^{(k)}(0)}{k!} = \frac{1}{k!}\left.\frac{d^kf}{dx^k}\right|_0$

k^{th} DERIVATIVE OF f

EVALUATED AT $x=0$

FACTORIAL

TAYLOR SERIES

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k = f(0) + \left.\frac{df}{dx}\right|_0 x$$

$$1 \qquad 1$$

CHECK

$$f(x) = e^x$$

$$e^x \xrightarrow{\frac{d}{dx}} e^x \xrightarrow{\frac{d}{dx}} e^x \xrightarrow{\frac{d}{dx}} e^x$$

$$= 1 + x + \frac{1}{2!}$$

$$= e^x$$