TEACHING FRESHMAN SCIENCE USING AGENT-BASED COMPUTATIONAL LABORATORIES

Drs. George Shiflet and Angela Shiflet
Wofford College

SIAM CSE
March 17, 2015

Computational science integral to science

Computational science integral to science

- They even have entire conferences on computational science!

Robert Harrison, director of Joint Institute for Computational Sciences at U. TN

- "If you look at **students** coming into our graduate program from the undergraduate world, **those that haven't already had some exposure to computation**, such as thinking algorithmically, solving problems on the computer, and the little bits of applied math that you need to understand all of that, …have **lost a year or two of productivity at the graduate level**. But it's not only the undergraduate students coming into graduate school that have this issue; it's also our undergrads going off into the larger world. **Industry and** many other aspects of the **commercial world use simulation and computation** in diverse ways"

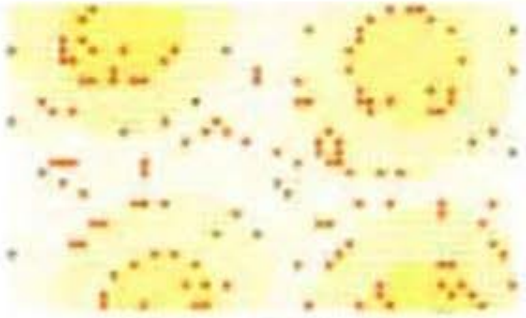
Course: Modeling and Simulation for the Sciences (COSC/Math 201)

Course: Modeling and Simulation for the Sciences (COSC/Math 201)

- Prerequisite: Calculus I
- Majors in biology, chemistry, computer science, environmental studies, mathematics, physics, psychology
- Modeling and Simulation for the Sciences (COSC/MATH 201)
  - system dynamics modeling (about 4.5 weeks)
  - simulation methods and error (about 1.5 weeks)
  - empirical modeling (about 1.5 weeks)
  - cellular automaton simulations (about 4.5 weeks)
  - **last week: agent-based modeling as it compares to other methods**

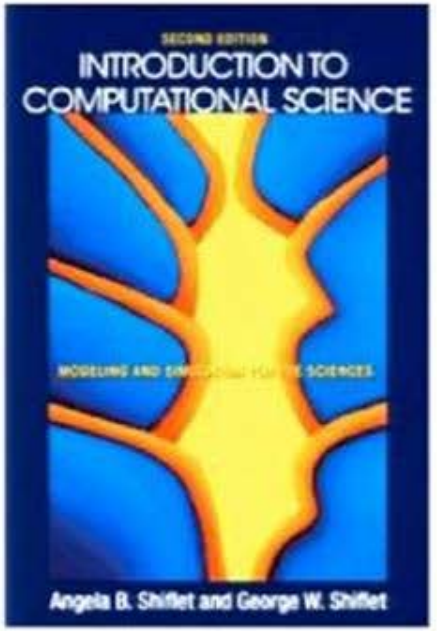
Agent-Based Models

- Simulate interactions between *agents*
- Agent's behavior governed by set of rules
- Agents act at any point in time according to their own situation, environment, and their rules of behavior
- Actions **not** based on some overarching assumption of equilibrium
- Agents interact directly with other agents
  - Conduct likely changed by interaction



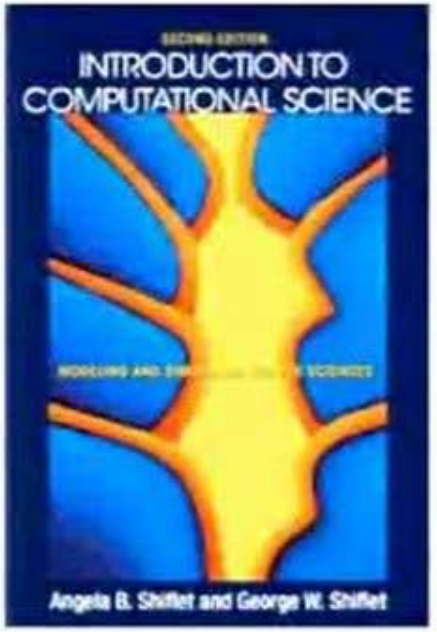
www.gazette.gmu.edu

Text


SECOND EDITION
INTRODUCTION TO
COMPUTATIONAL SCIENCE
Angela B. Shiflet and George W. Shiflet

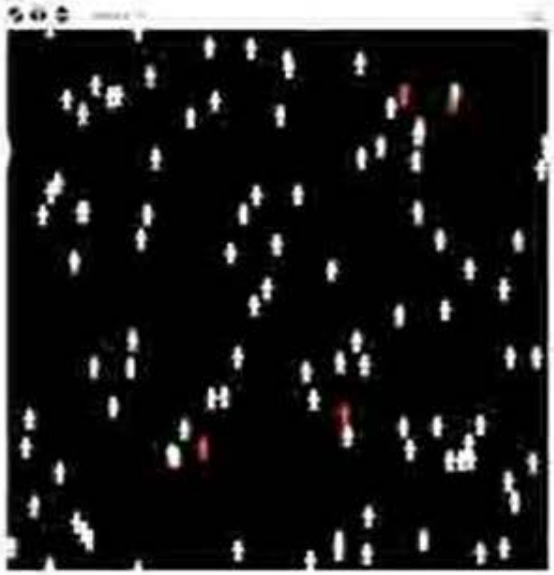
Text

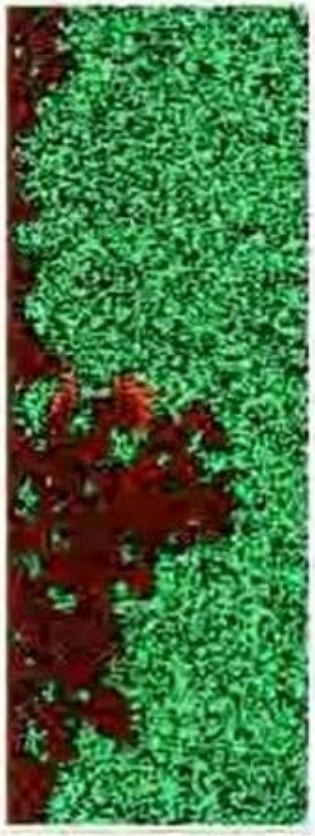
- *Introduction to Computational Science: Modeling and Simulation for the Sciences, 2nd Edition*
  - Princeton University Press, 2014
- http://wofford-ecs.org/IntroComputationalScience/
  - files & tutorials in various tools
- New to 2nd Edition (2014)
  - **Chapter on "Agent-Based Models"**
    - On website: 4 NetLogo tutorials & 4 AgentSheets totorials
  - 10 additional project modules
  - Chapter on "Matrix Models"
  - HPC materials

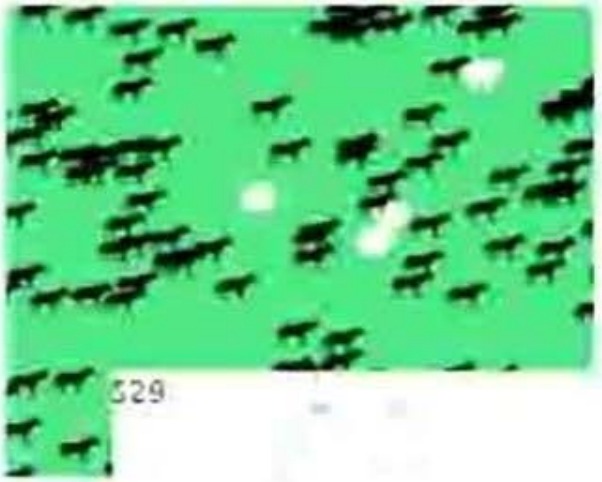


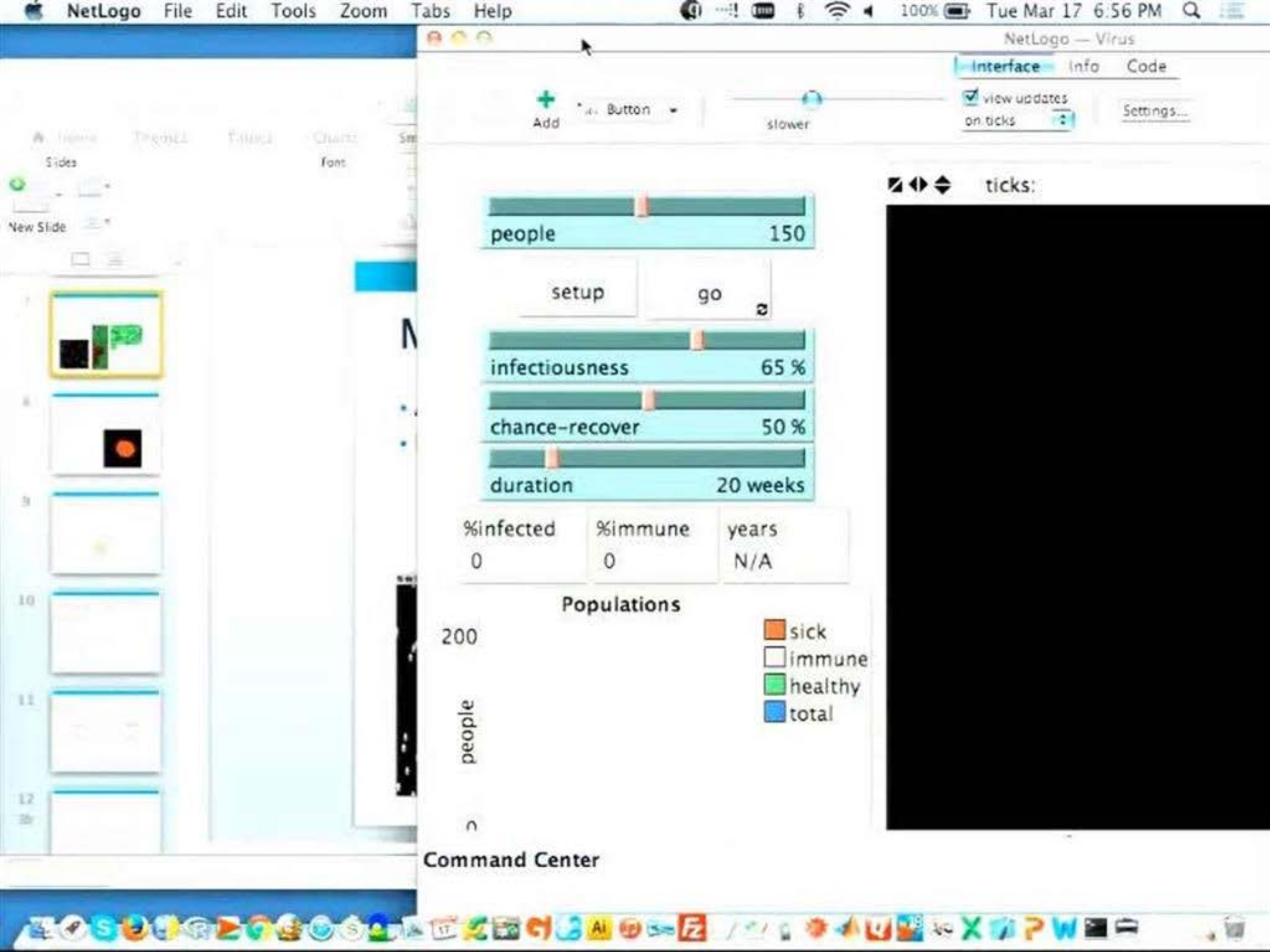
Monday's 50-minute class in ABM

- Applications from earlier in demonstrated, compared
- NetLogo
  - Interface
  - Info
  - Code








NetLogo File Edit Tools Zoom Tabs Help
Tue Mar 17 6:56 PM
NetLogo — Virus
Interface Info Code
Add
Button
slower
view updates
on ticks
Settings...
ticks:
people 150
setup
go
infectiousness 65 %
chance-recover 50 %
duration 20 weeks
%infected
0
%immune
0
years
N/A
Populations
200
people
0
sick
immune
healthy
total
Command Center

NetLogo File Edit Tools Zoom Tabs Help 100% Tue Mar 17 6:56 PM

NetLogo — Virus

Interface Info Code

Add Button slower view updates on ticks Settings...

people 150

setup go

infectiousness 65 %

chance-recover 50 %

duration 20 weeks

%infected	%immune	years
0	0	N/A

Populations

200

people

0

sick
immune
healthy
total

ticks:

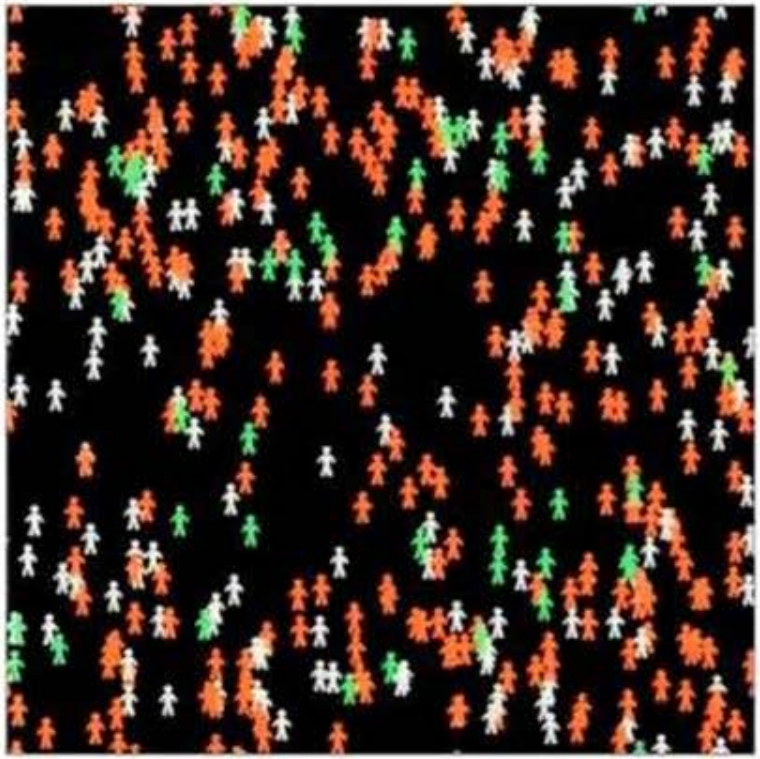
3D

Command Center

NetLogo File Edit Tools Zoom Tabs Help 100% Tue Mar 17 6:56 PM

Models Library

- Sample Models
  - Art
  - Biology
    - AIDS
    - Ant Lines
    - Ants
    - Autumn
    - Daisyworld
    - Disease Solo
    - Evolution
    - Fireflies
    - Flocking
    - Flocking Vee Formations
    - Fur
    - Heatbugs
    - Membrane Formation
    - Moths
    - Muscle Development
    - Rabbits Grass Weeds
    - Shepherds
    - Simple Birth Rates
    - Slime
    - Sunflower
    - Sunflower Emergent
    - Termites
    - Tumor
    - Virus
    - Wolf Sheep Predation
  - (unverified)
- Chemistry & Physics
- Computer Science



Virus

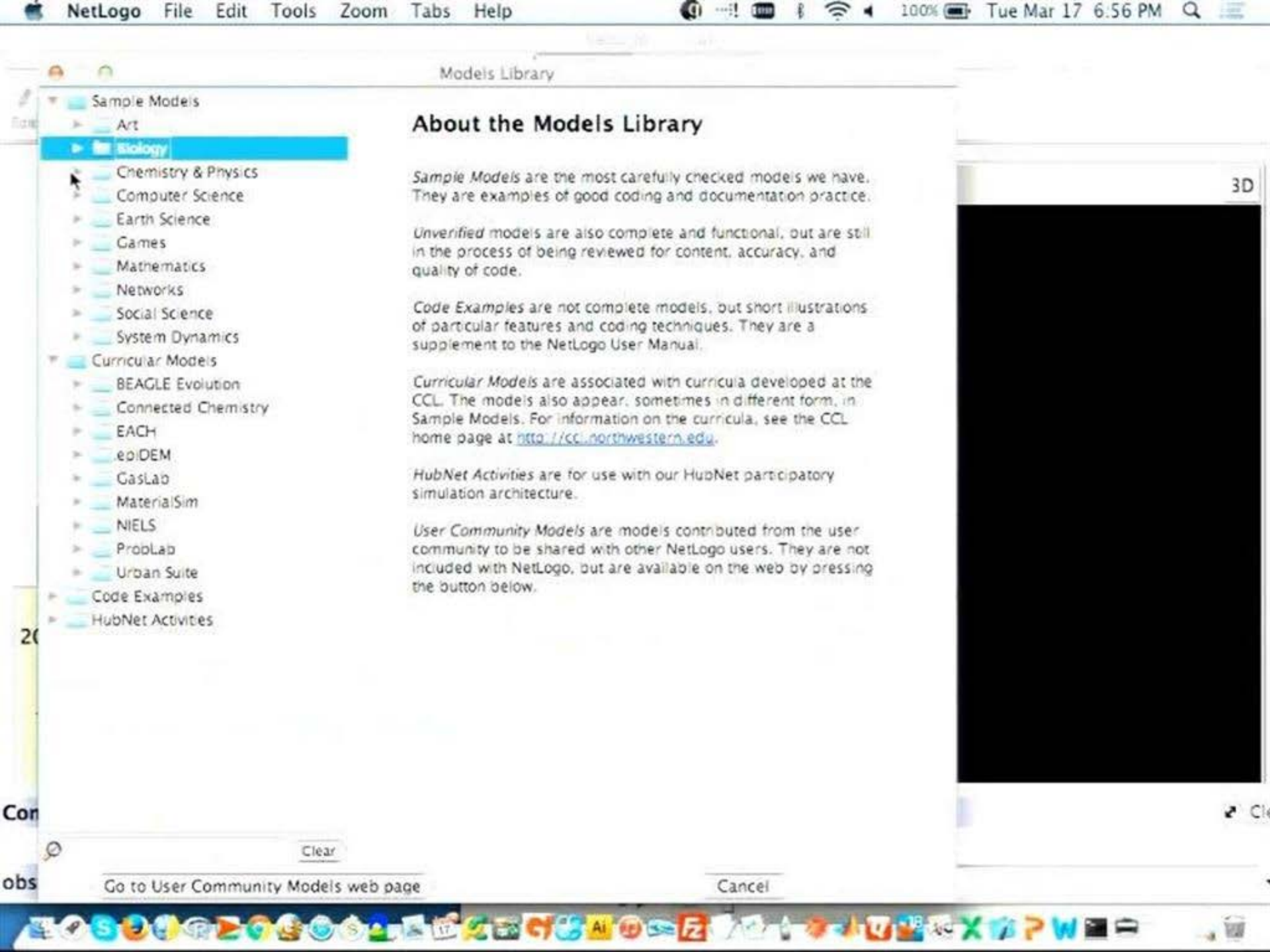
This model simulates the transmission and perpetuation of a virus in a human population.

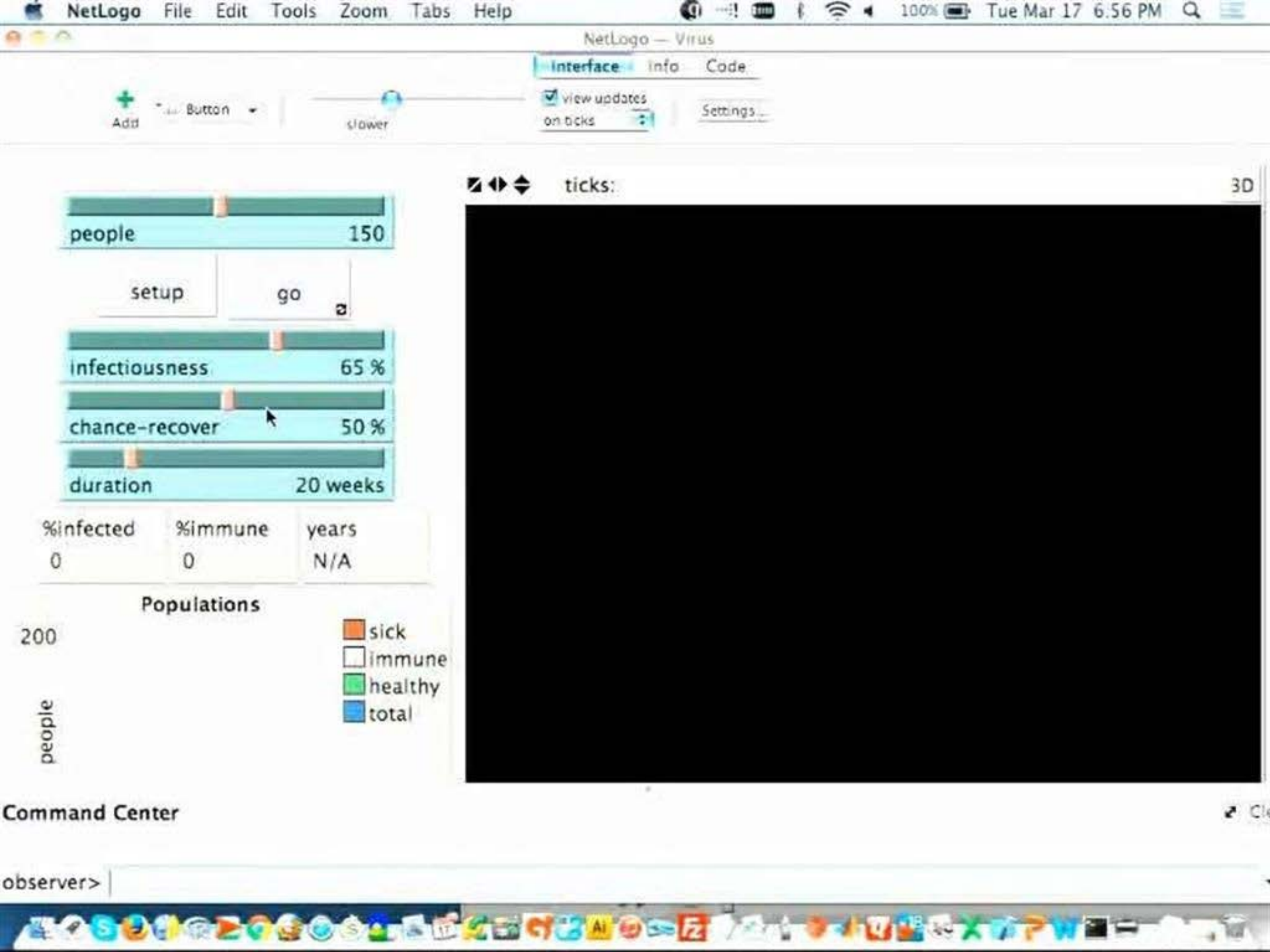
Clear

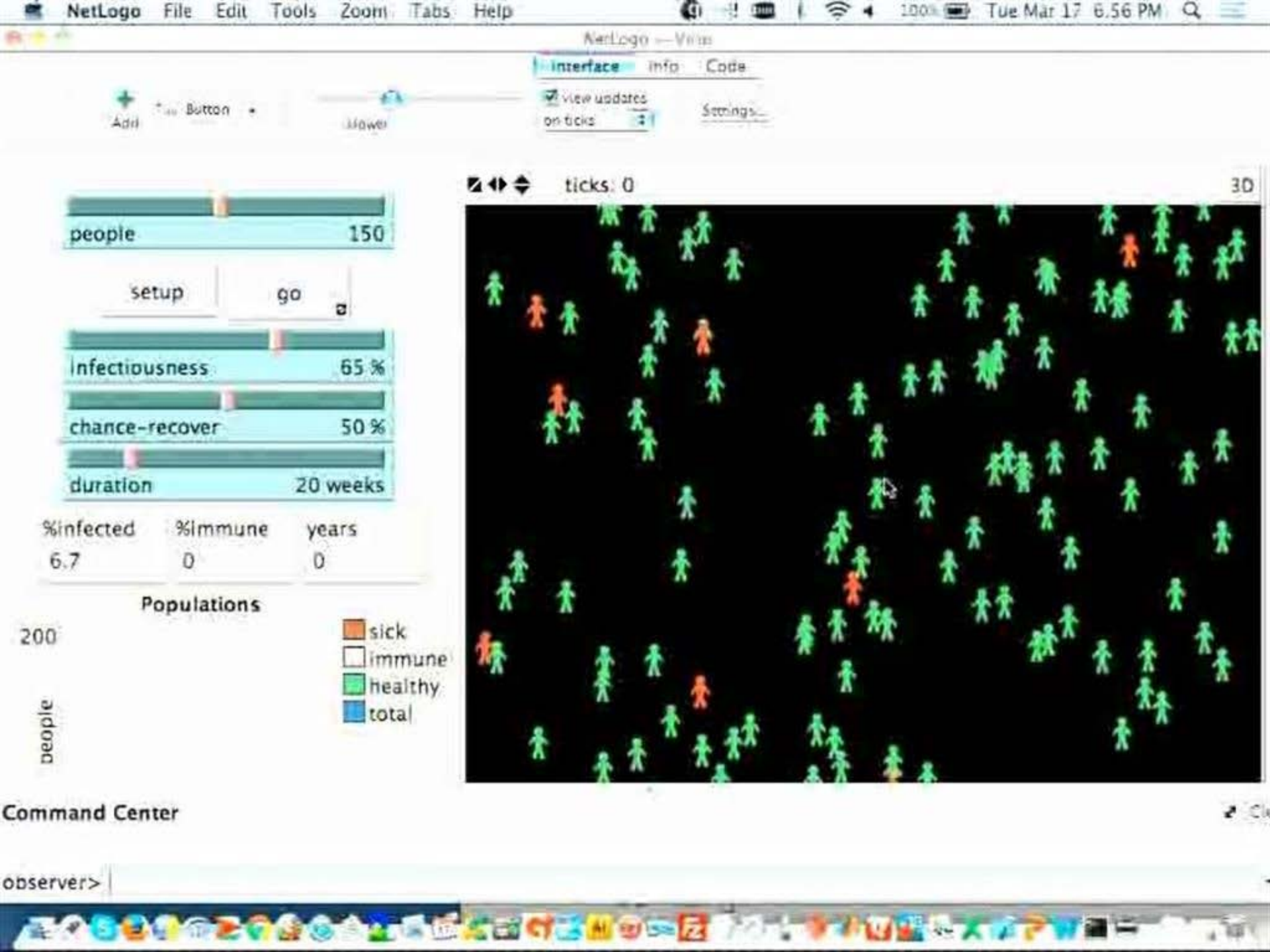
Go to User Community Models web page

Cancel Open

3D


NetLogo File Edit Tools Zoom Tabs Help
Tue Mar 17 6:56 PM
Models Library
Sample Models
Art
Biology
Chemistry & Physics
Computer Science
Earth Science
Games
Mathematics
Networks
Social Science
System Dynamics
Curricular Models
BEAGLE Evolution
Connected Chemistry
EACH
epiDEM
GasLab
MaterialSim
NIELS
ProbLab
Urban Suite
Code Examples
HubNet Activities
About the Models Library
Sample Models are the most carefully checked models we have. They are examples of good coding and documentation practice.
Unverified models are also complete and functional, but are still in the process of being reviewed for content, accuracy, and quality of code.
Code Examples are not complete models, but short illustrations of particular features and coding techniques. They are a supplement to the NetLogo User Manual.
Curricular Models are associated with curricula developed at the CCL. The models also appear, sometimes in different form, in Sample Models. For information on the curricula, see the CCL home page at http://ccl.northwestern.edu.
HubNet Activities are for use with our HubNet participatory simulation architecture.
User Community Models are models contributed from the user community to be shared with other NetLogo users. They are not included with NetLogo, but are available on the web by pressing the button below.
Clear
Go to User Community Models web page
Cancel
3D


NetLogo File Edit Tools Zoom Tabs Help
Tue Mar 17 6:56 PM
NetLogo — Virus
Interface Info Code
Add
Button
slower
view updates
on ticks
Settings...
people 150
setup
go
infectiousness 65 %
chance-recover 50 %
duration 20 weeks
%infected
0
%immune
0
years
N/A
Populations
200
people
sick
immune
healthy
total
ticks:
3D
Command Center
observer>


NetLogo File Edit Tools Zoom Tabs Help
Tue Mar 17 6:56 PM
NetLogo — Virus
Interface Info Code
Add Button
Slider
View updates
on ticks
Settings...
ticks: 0
3D
people 150
setup
go
infectiousness 65 %
chance-recover 50 %
duration 20 weeks
%infected
6.7
%immune
0
years
0
Populations
200
people
sick
immune
healthy
total
Command Center
observer>

NetLogo File Edit Tools Zoom Tabs Help

Tue Mar 17 6:57 PM

NetLogo — Virus

Interface Info Code

Add Button Slower

view updates on ticks Settings...

people 150

setup go

infectiousness 65 %

chance-recover 50 %

duration 20 weeks

%infected	%immune	years
26.3	49	1.7

Populations

536

people

0

sick
immune
healthy
total

Command Center

observer>

WHAT IS IT?

This model simulates the transmission and perpetuation of a virus in a human population.

Ecological biologists have suggested a number of factors which may influence the survival of a directly transmitted virus within a population. (Yorke, et al. "Seasonality and the requirements for perpetuation and eradication of viruses in populations." Journal of Epidemiology, volume 109, pages 103-123)

HOW IT WORKS

The model is initialized with 150 people, of which 10 are infected. People move randomly about the world in one of three states: healthy but susceptible to infection (green), sick and infectious (red), and healthy and immune (gray). People may die of infection or old age. When the population dips below the environment's "carrying capacity" (set at 700 in this model) healthy people may reproduce healthy and susceptible offspring.

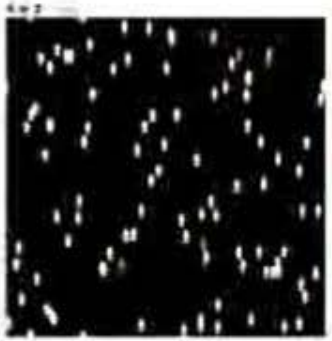
Some of these factors are summarized below with an explanation of how each one is treated in this model.

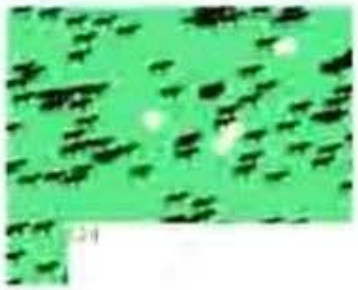
The density of the population

```
turtles-own
  [ sick?          ;; if true, the turtle is infectious
    immune?        ;; if true, the turtle can't be infected
    sick-count     ;; how long the turtle has been infectious
    age ]          ;; how many weeks old the turtle is

globals
[
  %infected              ;; what % of the population is infectious
  %immune                ;; what % of the population is immune
  lifespan               ;; the average lifespan of a turtle
  average-offspring      ;; the average number of offspring a turtle could have
  carrying-capacity      ;; the number of turtles that can be in the world at on
]

;; The setup is divided into three subroutines
to setup
  clear-all
  setup-constants
  setup-turtles
  update-global-variables
```

Monday's 50-minute class in ABM

- Applications from earlier in demonstrated, compared
- NetLogo
  - Interface
  - Info
  - Code



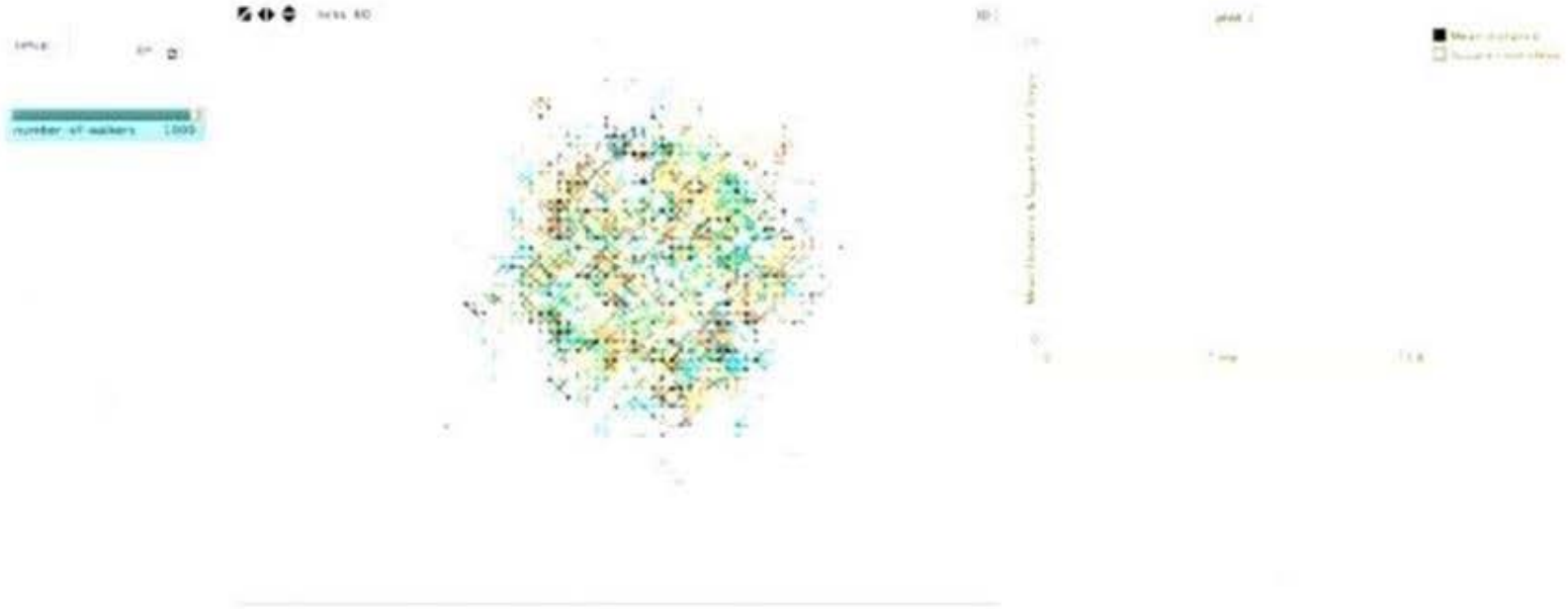


ABM Tutorial 1

- started Tutorial 1 in class, finished before Wednesday
- develop AB simulation of unconstrained growth of bacteria
- step-by-step with quick review questions

ABM Tutorial 2

- random-walk simulation with up to 1000 walkers
- plotted average distance traveled by walkers and square root of number of steps (*n*) versus time



Results for agent-based modeling at end of Modeling and Simulation course

- **very successful**
  - **tutorial** completion
  - improved **scores** on tests of modeling characteristics
  - **reports** of existing models
  - **questionnaire** answers
  - **another major simulation technique** that is having increasing utility in natural, physical, and social sciences
  - conduit for **comparison** of various modeling and simulation techniques

From
computational science education
to
computational science education

New course at Wofford College

New course at Wofford College

- Scientific Investigations Using Computation (COSC 150)
- Employ computational approaches to investigate scientific questions
- Explore important science concepts
- Using computational tools, implement scientific method to gain better understanding of natural world
- Satisfies one semester of BA science requirement
- Designed so that faculty member of any traditional science or computer science department can teach

Collection of self-contained, science teaching modules

- Bundle for variety of introductory college (or high school) science courses
- Module contains background material
- Quick review questions
- Points of Inquiry
  - Take-home projects
- Pertinent scientific literature

Computational Laboratories

Computational Laboratories

- Exploration and experimentation using free computational tools
  - NetLogo
  - Excel or other spreadsheet software
  - Molecular Biology Workbench
  - Gapminder
- Students
  - Explore model
  - Adjust parameters
  - Answer questions
  - Make observations
  - Formulate connections with the module material
  - Draw conclusions

This semester

This semester

- Tuesday-Thursday class (1 hr, 20 min each)
- Monday lab (3 hr) with 2 TAs
- Week 1 Lab
  - Getting Started Using NetLogo
- Week 1 Classes
  - Overview of computational science
  - In pairs, report on a NetLogo model
  - Write paragraph about another model
  - Assign "Carbon Cycle" module
  - Practice quizzes online
    - 1 version with questions in order, immediate feedback
    - Another version with questions in random order, immediate feedback

Week 2

Week 2

- Week 2 Lab
  - Getting Started with NetLogo Programming
- Week 2 Classes
  - "Carbon Cycle" quiz on Moodle
    - Automatically graded
  - Calculate carbon footprint with guided questions
    - http://www.epa.gov/climatechange/ghgemissions/ind-calculator.html
  - Points of Inquiry – 10-min team PowerPoint presentations
    - What city can be/has been done by city, farmers, government, construction
    - Pros and cons of carbon credits and biofuels
    - Deforestation of rainforests
  - Assign "Over Our Heads? Atmospheric Carbon and Climate Change"
  - Assign pre-lab for next lab

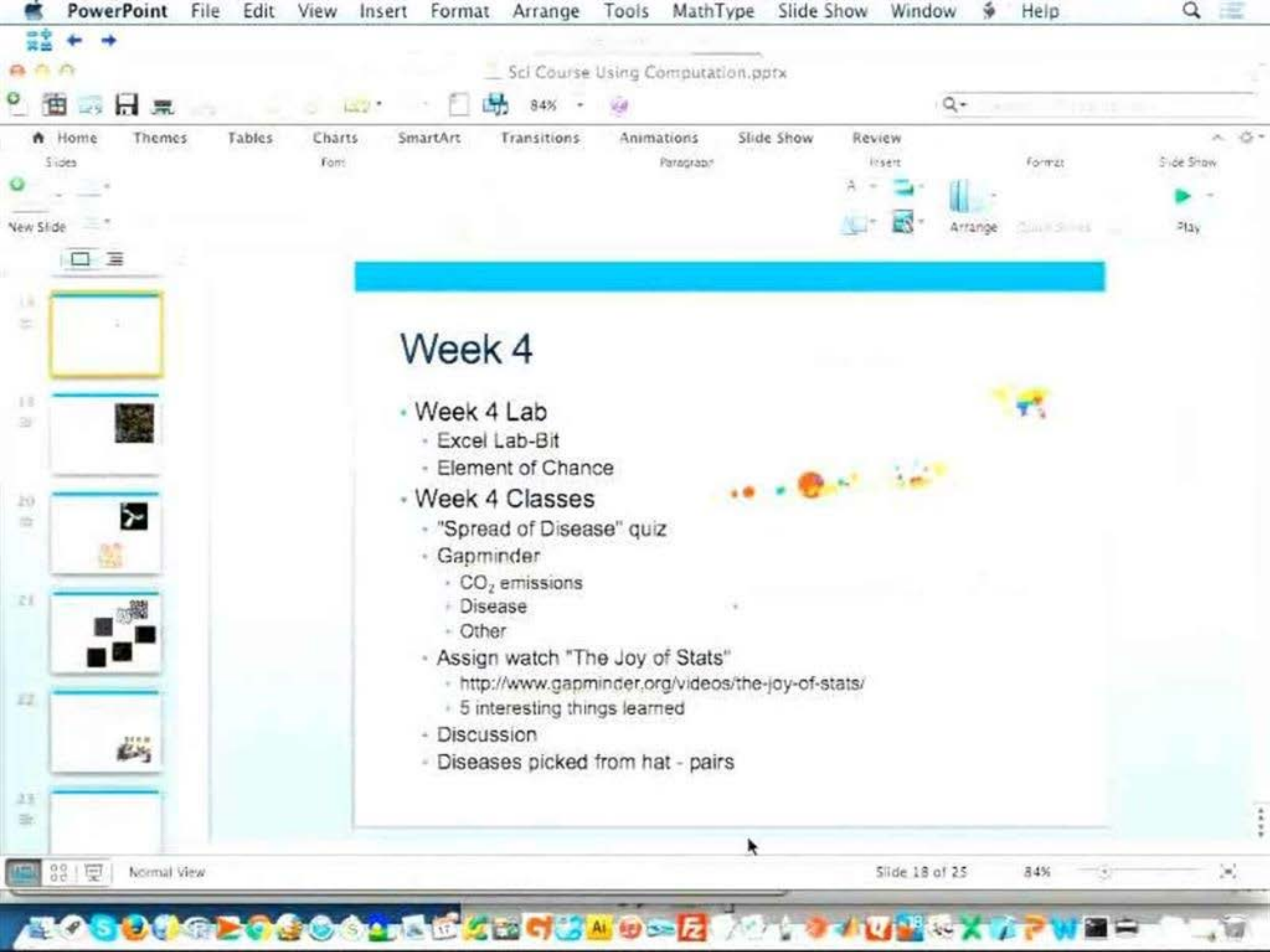
Week 3

- Week 3 Lab
  - Carbon Dioxide and Global Warming

Week 3

- Week 3 Lab
  - Carbon Dioxide and Global Warming
- Week 3 Classes
  - "Global Warming" quiz on Moodle
  - Assign one-page paper from PoI
  - Talk on "Measuring Climate Change"
    - Paragraph
  - Assign "Spread of Disease: The Sickening Consequences"
  - Assign pre-lab
  - Assign update individually PowerPoint slides from last week

Week 4

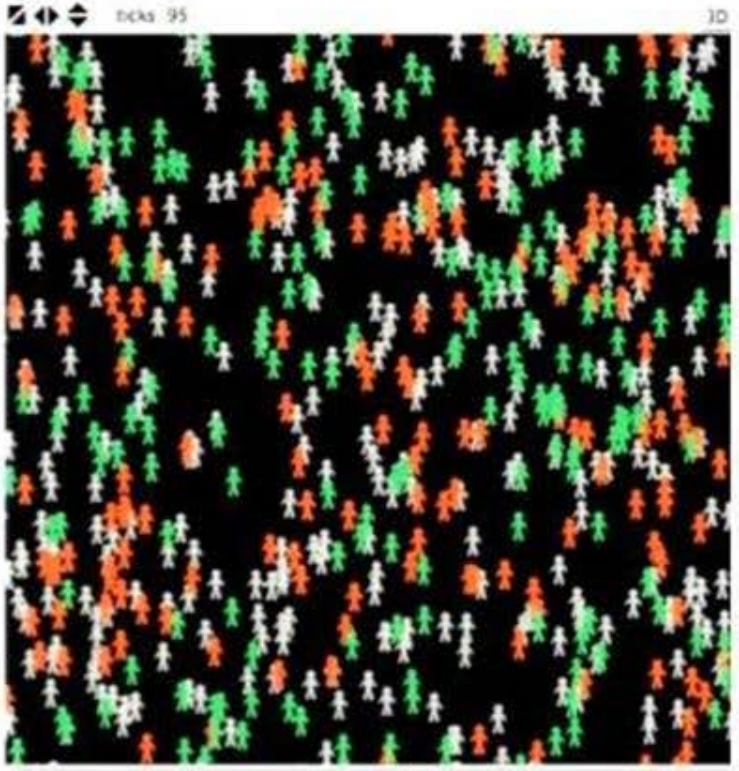

PowerPoint File Edit View Insert Format Arrange Tools MathType Slide Show Window Help
Sci Course Using Computation.pptx
Home Themes Tables Charts SmartArt Transitions Animations Slide Show Review
New Slide
Arrange
Play
Week 4
Week 4 Lab
Excel Lab-Bit
Element of Chance
Week 4 Classes
"Spread of Disease" quiz
Gapminder
CO_2 emissions
Disease
Other
Assign watch "The Joy of Stats"
http://www.gapminder.org/videos/the-joy-of-stats/
5 interesting things learned
Discussion
Diseases picked from hat - pairs
Normal View
Slide 18 of 25
84%

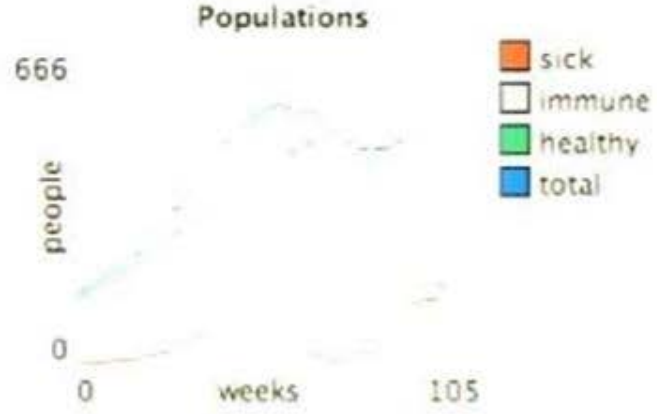
Week 4

- Week 4 Lab
  - Excel Lab-Bit
  - Element of Chance
- Week 4 Classes
  - "Spread of Disease" quiz
  - Gapminder
    - CO_2 emissions
    - Disease
    - Other
  - Assign watch "The Joy of Stats"
    - http://www.gapminder.org/videos/the-joy-of-stats/
    - 5 interesting things learned
  - Discussion
  - Diseases picked from hat - pairs

Week 4

Weeks 5 & 6

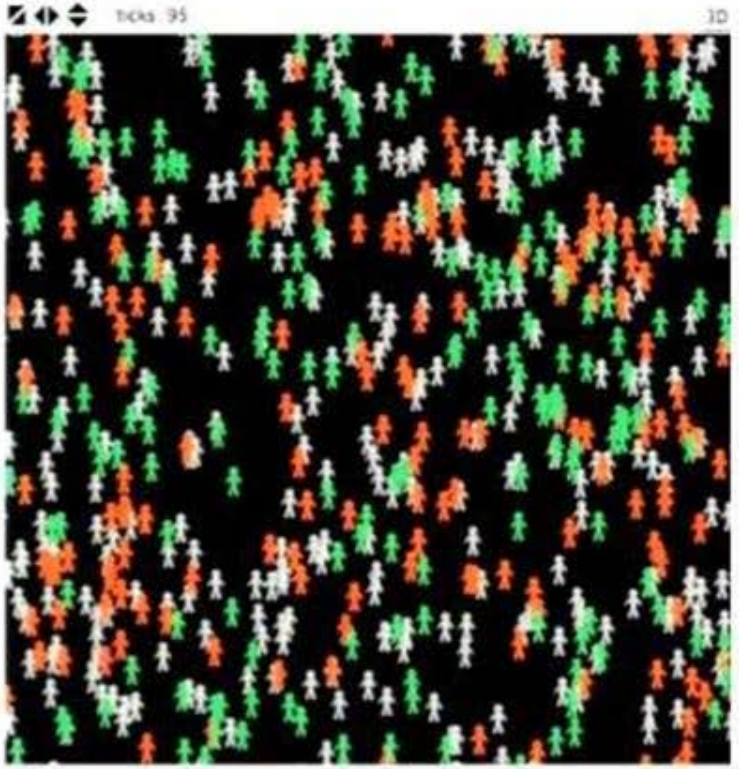

ticks 95
3D

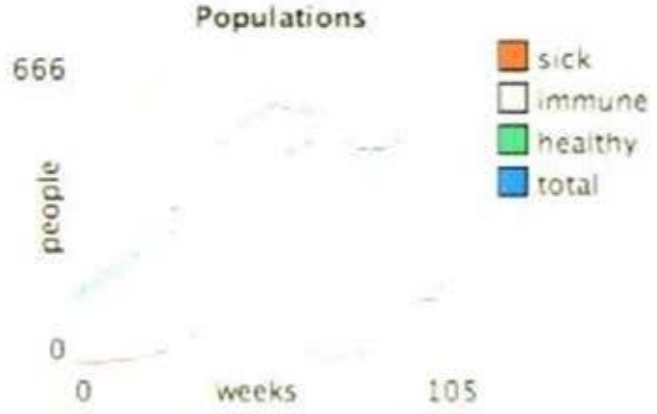

Populations
666
people
0
0
weeks
105
sick
immune
healthy
total

Week 4

- Week 4 Lab
  - Excel Lab-Bit
  - Element of Chance
- Week 4 Classes
  - "Spread of Disease" quiz
  - Gapminder
    - CO_2 emissions
    - Disease
    - Other
  - Assign watch "The Joy of Stats"
    - http://www.gapminder.org/videos/the-joy-of-stats/
    - 5 interesting things learned
  - Discussion
  - Diseases picked from hat - pairs

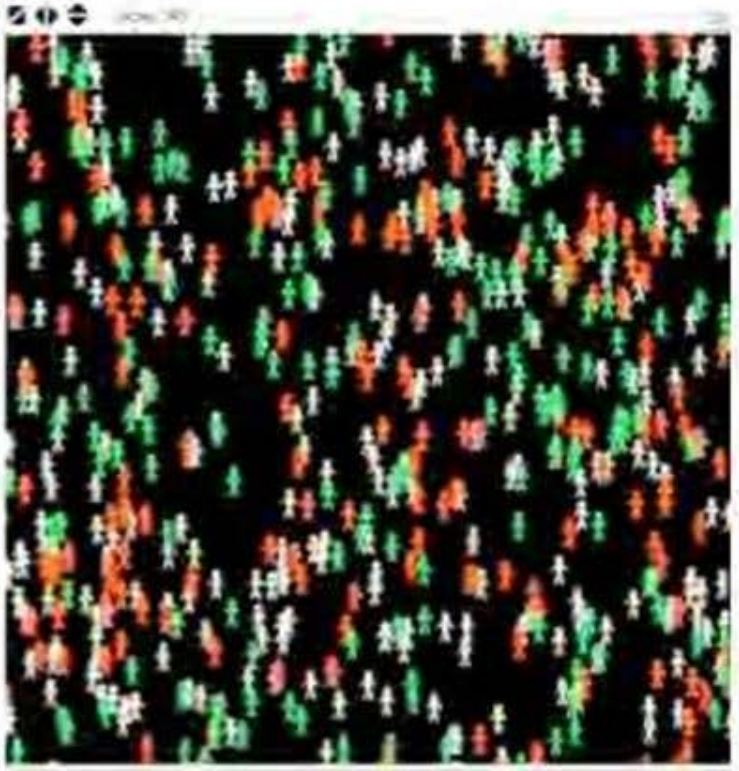
Weeks 5 & 6

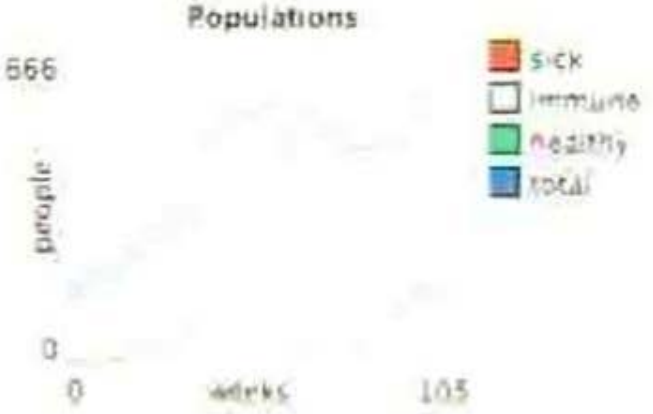

ticks: 95
3D


Populations
666
people
0
0
weeks
105
sick
immune
healthy
total

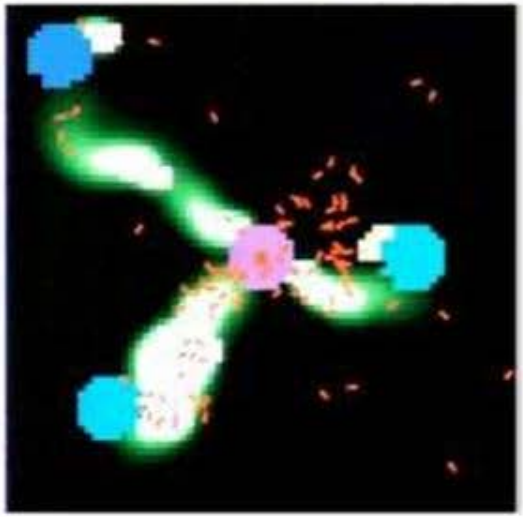
Weeks 5 & 6

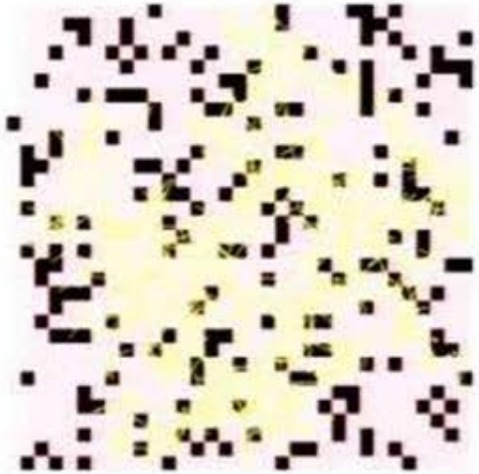
- Week 5 Lab
  - Modeling spread of disease
- Week 5 Classes
  - 5-minute presentation on disease
  - Start working on modeling disease by making adjustments to *Virus.nlogo*
- Week 6 Lab
  - Continue working on modeling disease
  - Individual report due following week
- Week 6 Classes
  - Quiz on "Getting the Message - Communication for Life"





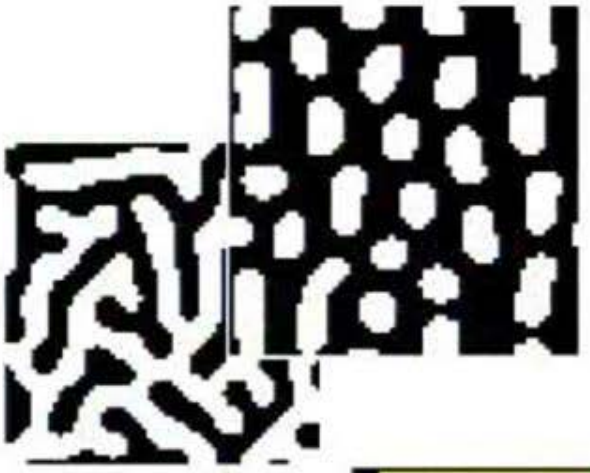
Weeks 7 - 8

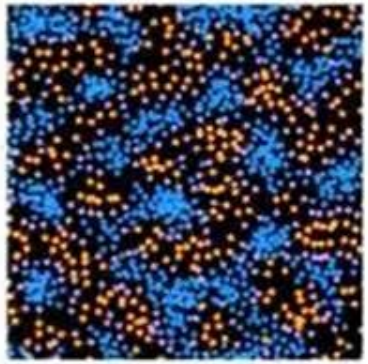


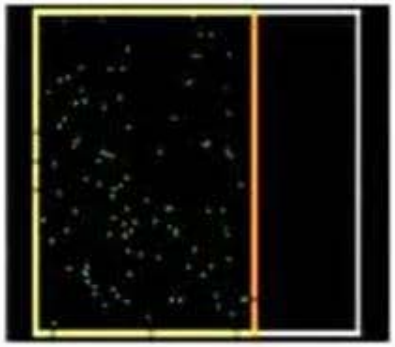


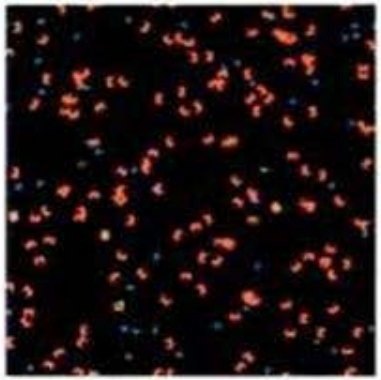
Remaining topics

- Patterns
- Membranes
- Gas Laws
- Chemical Kinetics
- Enzyme Kinetics
- Final projects
  - Develop module
  - Develop model









6-week evaluation

1 (strongly disagree) to 5 (strongly agree)

- I have a better understanding of computational science from taking the course.
  - 3.2
- I understand the science in the modules.
  - 3.8
- The modules are clear and readable.
  - 3.7
- I understand the laboratories.
  - 3.4
- The quizzes are reasonable.
  - 4.3
- The class time is meaningful.
  - 3.8

Evaluation comments & course adjustments

Evaluation comments & course adjustments

- More connection with computational science during class
  - Adjustment: After quiz on Tuesday, students investigate computational science topic related to Monday's lab. Discuss
  - Adjustment: Look for more tools, such as Gapminder
- More study of programming
  - Misunderstanding of course will change with time
  - Adjustment: Code review Tuesday about Monday's lab
  - Adjustment: Small programming assignments related to review
  - Adjustment: More discussion of code before model development, such as modeling particular disease

Conclusions - Scientific Investigations Using Computation

References

- Gapminder, http://www.gapminder.com
- Introduction to Computational Science (2014). Website associated with *Introduction to Computational Science: Modeling and Simulation for the Sciences, 2nd Edition*. http://wofford-ecs.org/IntroComputationalScience/
- "Joy of Stats," http://www.gapminder.org/videos/the-joy-of-stats/
- NetLogo, http://ccl.northwestern.edu/netlogo/
- Shiflet, A. and G. Shiflet (2014). *Introduction to Computational Science: Modeling and Simulation for the Sciences, 2nd Edition*, Princeton University Press