Simulation

COS 323

Last Time

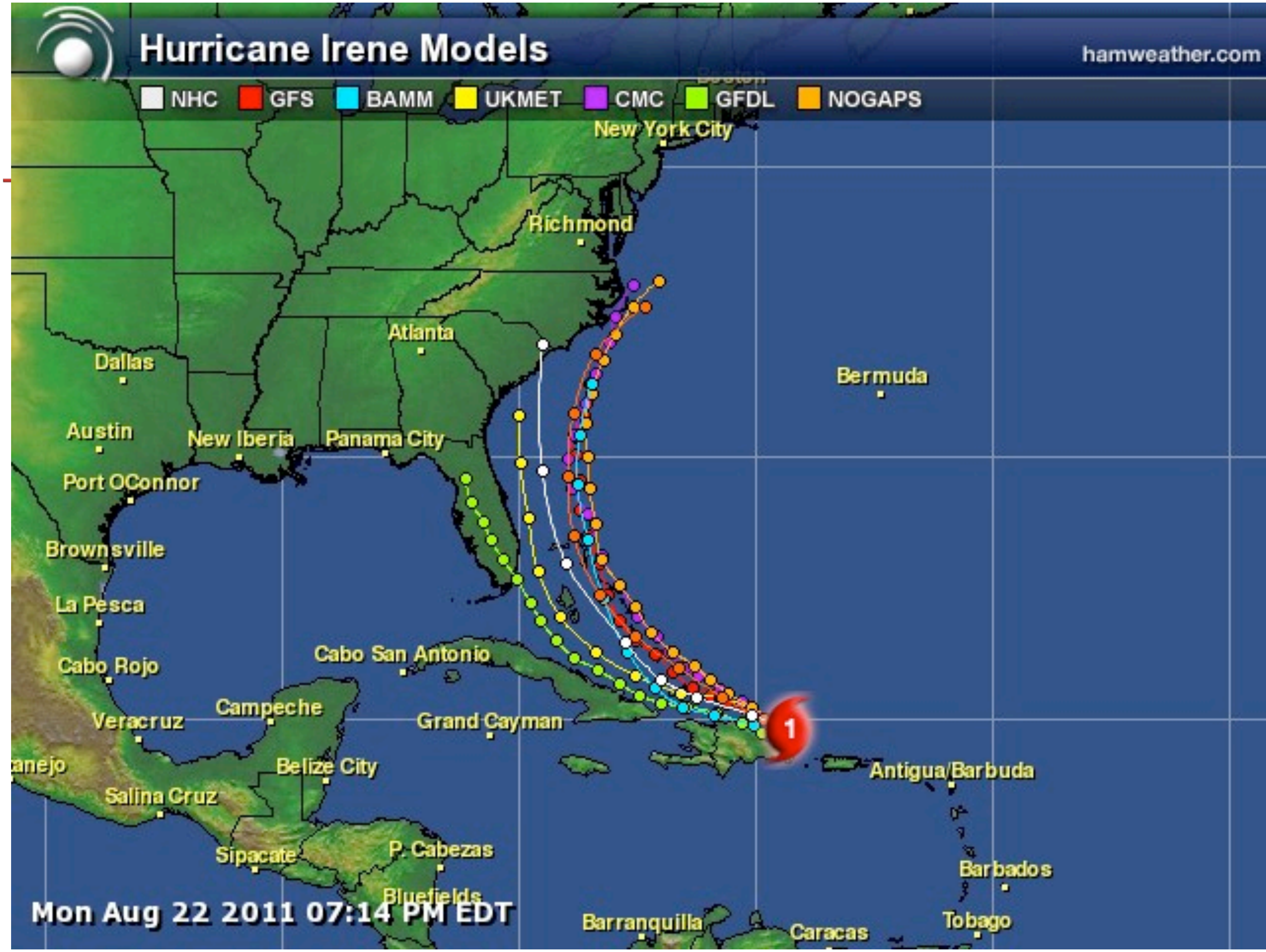
- Stability of ODEs
- Stability of PDEs
- Review of methods for solving large, sparse systems
- Multi-grid methods

Reminders

- Homework 4 due Tuesday
- Homework 5, final project proposal due Friday December **16**

Today

- Simulation examples
- Discrete event simulation
  - Time-driven and event-driven approaches, with examples
  - Cellular automata, microsimulation, agent-based simulation
- Population genetics overview



Hurricane Irene Models
hamweather.com
NHC
GFS
BAMM
UKMET
CMC
GFDL
NOGAPS
New York City
Richmond
Atlanta
Dallas
Bermuda
Austin
New Iberia
Panama City
Port OConnor
Brownsville
La Pesca
Cabo San Antonio
Cabo Rojo
Campeche
Veracruz
Grand Cayman
Belize City
Antigua/Barbuda
Salina Cruz
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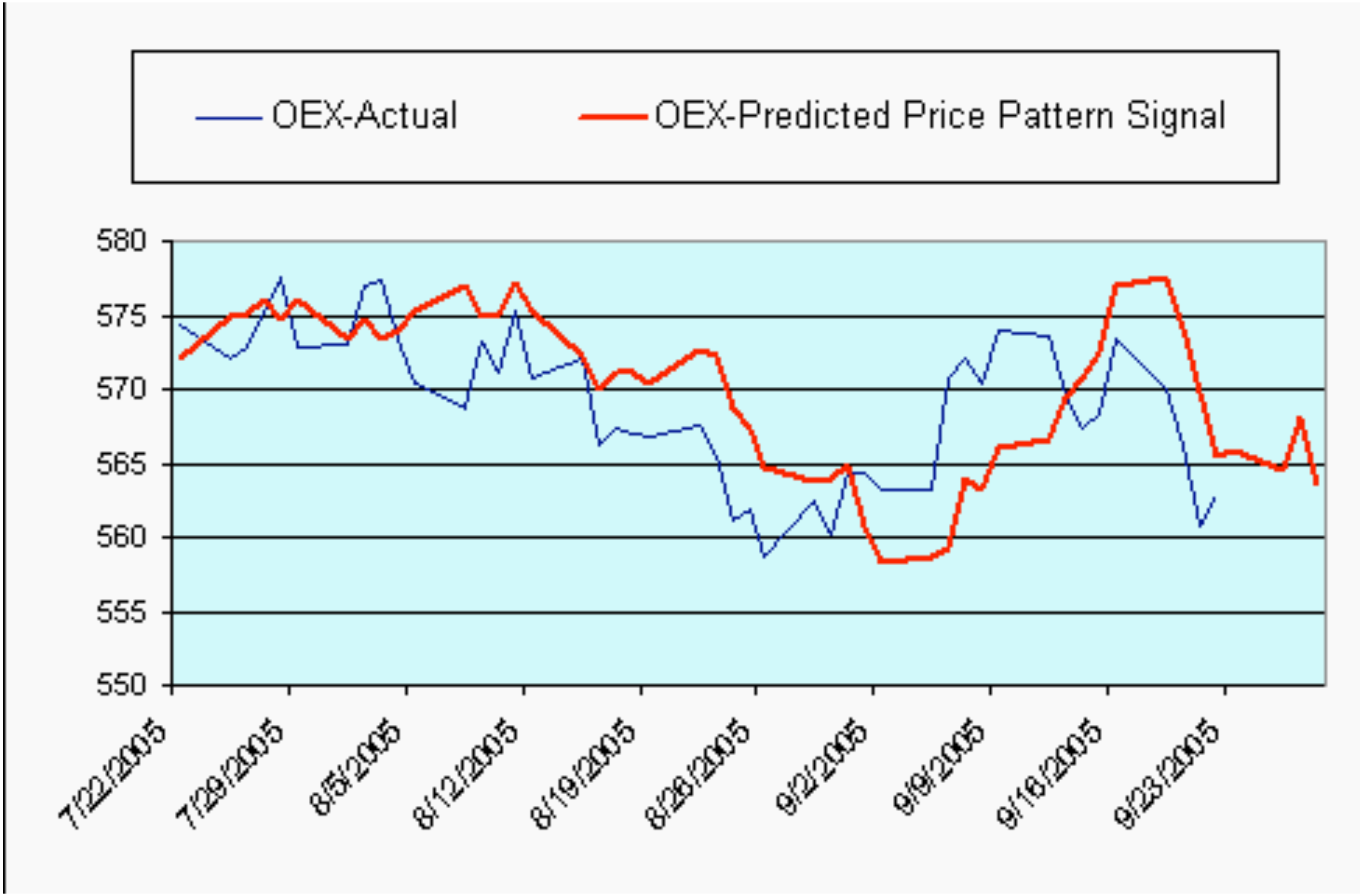
OEX-Actual
OEX-Predicted Price Pattern Signal
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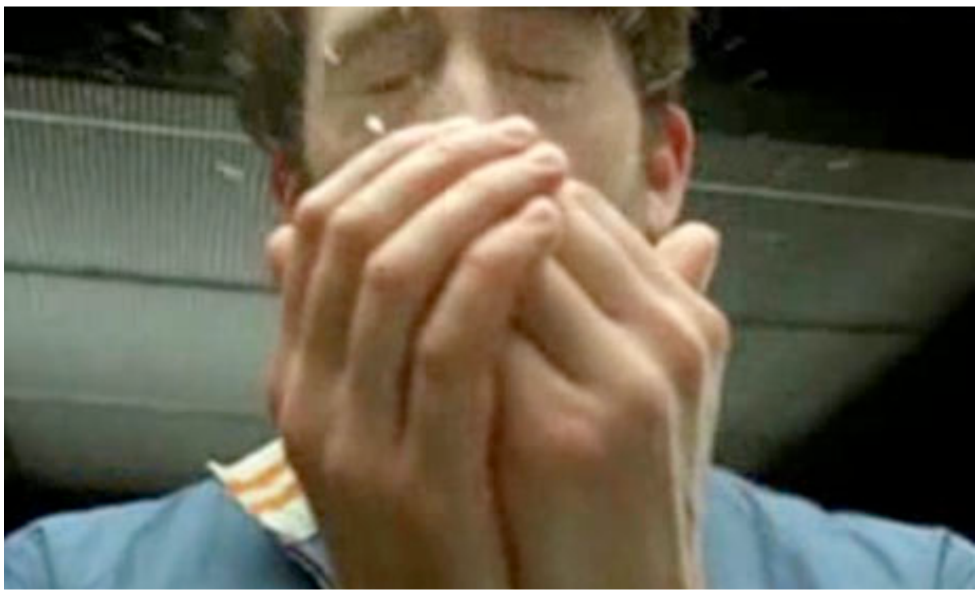


Why simulation?

- Make predictions or make decisions regarding complex phenomena or poorly-understood phenomena
- Test theories about how real systems work
- Explore consequences of changes to a system
- Train people to make better decisions or take correct actions
- …

Simulation

One program variable for each element in the system being simulated,

… as opposed to

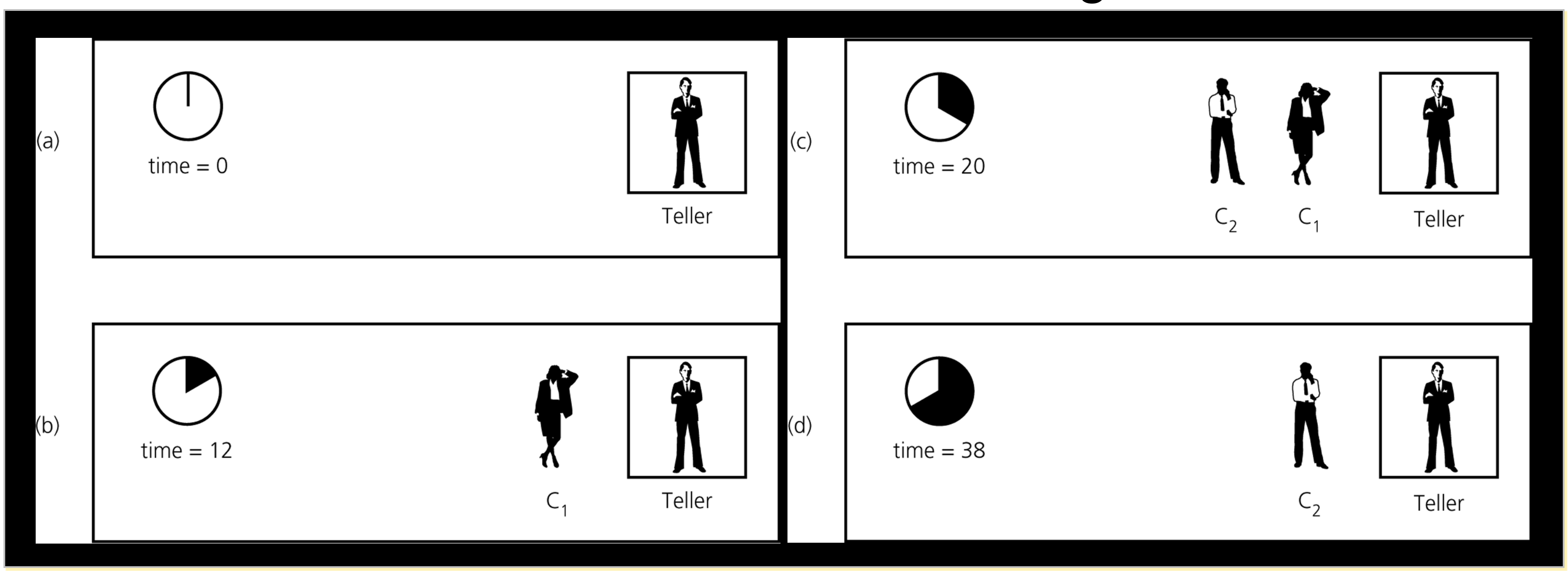
- analytical solution
- formulation of algebraic or differential equations

Approaches to Simulation

- Differential equation solvers can be thought of as conducting a *simulation* of a physical system
  - Advance through time
  - "Continuous" equations model change in state
- Some simulations are more "discrete":
  - Decisions, actions, events happen at discrete points in time

Discrete Event Simulation: Bank Teller Example

- Simple example: lines at the bank
  - Customers arrive at random times
  - Wait in line(s) until teller available
  - Conduct transaction of random length



Bank Teller

- Simple example: lines at the bank
  - Customers arrive at random times
  - Wait in line(s) until teller available
  - Conduct transaction of random length
- Simulate arbitrary phenomena
  (e.g. spike in customer rate during lunch)
- Goal: mean and variance of waiting times
  - As a function of customer rate, # tellers, # queues

Bank Teller

- *Time-driven* simulation:
  - A master clock increments time in fixed-length steps
  - At each step, compute probability of customer(s) arriving, determine whether any transactions finishing
    - e.g., probability of 2% that a new customer arrives at each time step
  - More accurate simulation with shorter time steps, but then have more steps when *nothing* happens

Bank Teller

- *Event-driven* simulation:
  - **Events** change system state:
    - New customer arrives
    - Teller finishes processing a customer
  - Compute times of events and put in a "future event list":
    - When will new customers arrive?
    - When new customer reaches teller, compute time that customer will finish.
  - Repeatedly process one event, then fast-forward until scheduled time of next event
  - Good accuracy and efficiency: automatically use time steps appropriate for how much is happening

Time-driven Example: Epidemics

The SIR Model

- W. O. Kermack and A. G. McKendrick, 1929
- susceptible: susceptible, not yet infected
- infected: infected and capable of spreading
- recovered / removed: recovered and immune

$$\frac{dS}{dt} = -\beta S I$$

$$\frac{dI}{dt} = \beta S I - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

Time-Driven Simulation: Epidemics

- [Dur95] R. Durrett, "Spatial Epidemic Models," in Epidemic Models: Their Structure and Relation to Data, D. Mollison (ed.), Cambridge University Press, Cambridge, U.K., 1995.

- Discrete-time, discrete-space, discrete-state

Durrett's Spatial SIR model

- Time, $t = 0, 1, 2, \ldots$
- Space: orthogonal (square) grid
- State: {susceptible, infected, removed}

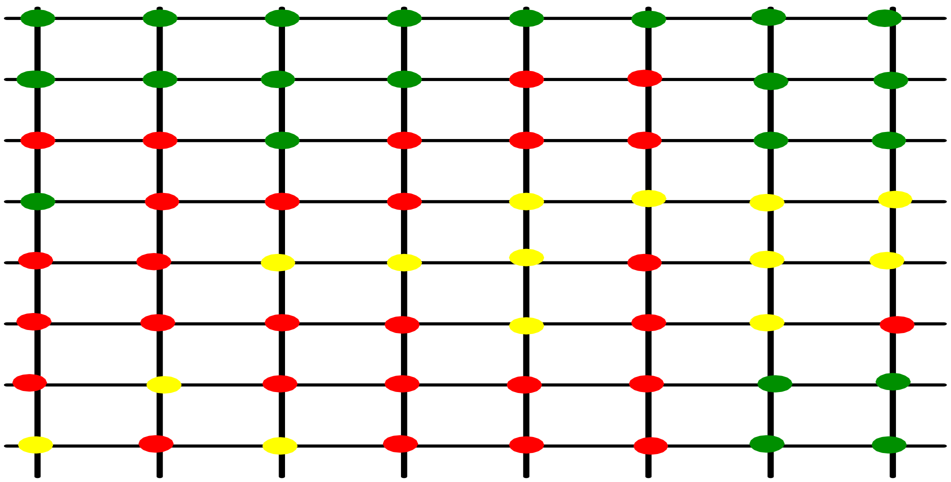
Rules tell us how to get from t to $t+1$ for each spatial location

Each site has 4 neighbors,

contains 0 or 1 individual

Durrett's Rules for Spatial SIR model

- Susceptible individuals become infected at rate proportional to the number of infected neighbors
- Infected individuals become healthy (removed) at a fixed rate δ
- Removed individuals become susceptible at a fixed rate α



Time, t = 0, 1, 2, …

Space: orthogonal (square) grid

State: {susceptible, infected, removed}

Simulation Results

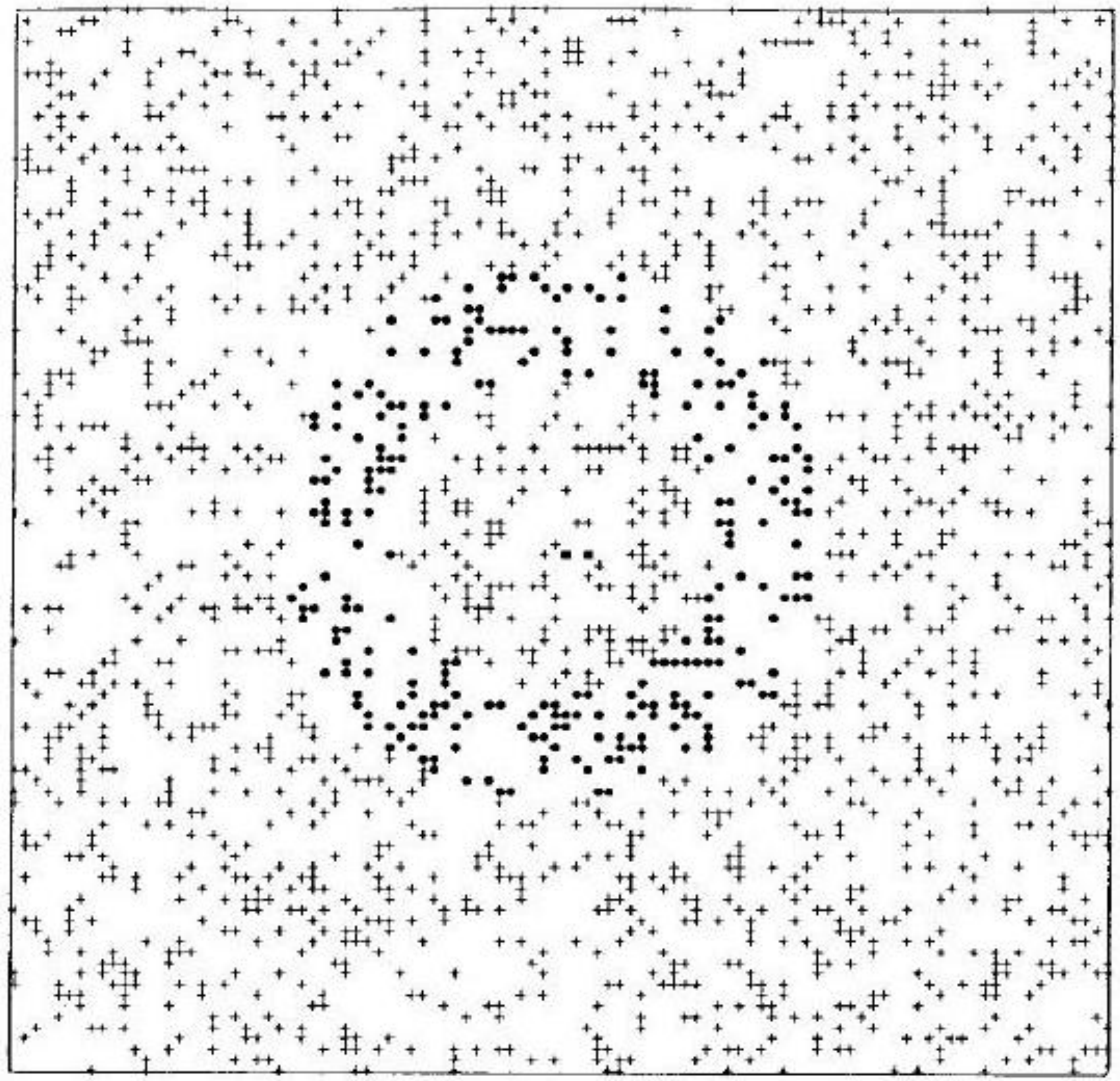
$\alpha = 0$: No return from removed; immunity is permanent. If δ, recovery rate, is large, epidemic dies out. If δ is less than some critical number, the epidemic spreads *linearly* and approaches a *fixed shape*.

→ Can be formulated and proven as a theorem!

$\alpha > 0$: behavior is more complicated

More recent work:

"Epidemic Thresholds and Vaccination in a Lattice Model of Disease Spread", C.J. Rhodes and R.M. Anderson, *Theoretical Population Biology* **52**, 101118 (1997) Article No. TP971323.



Note ring of vaccinated individuals.

The SZR model

- Susceptible
  - Can die naturally with parameter delta (become Removed)
  - Can become zombie-infected with parameter beta
- Zombie
  - Can be killed by human with parameter alpha (become removed)
- Removed
  - Removed humans can be resurrected into zombies with parameter zeta

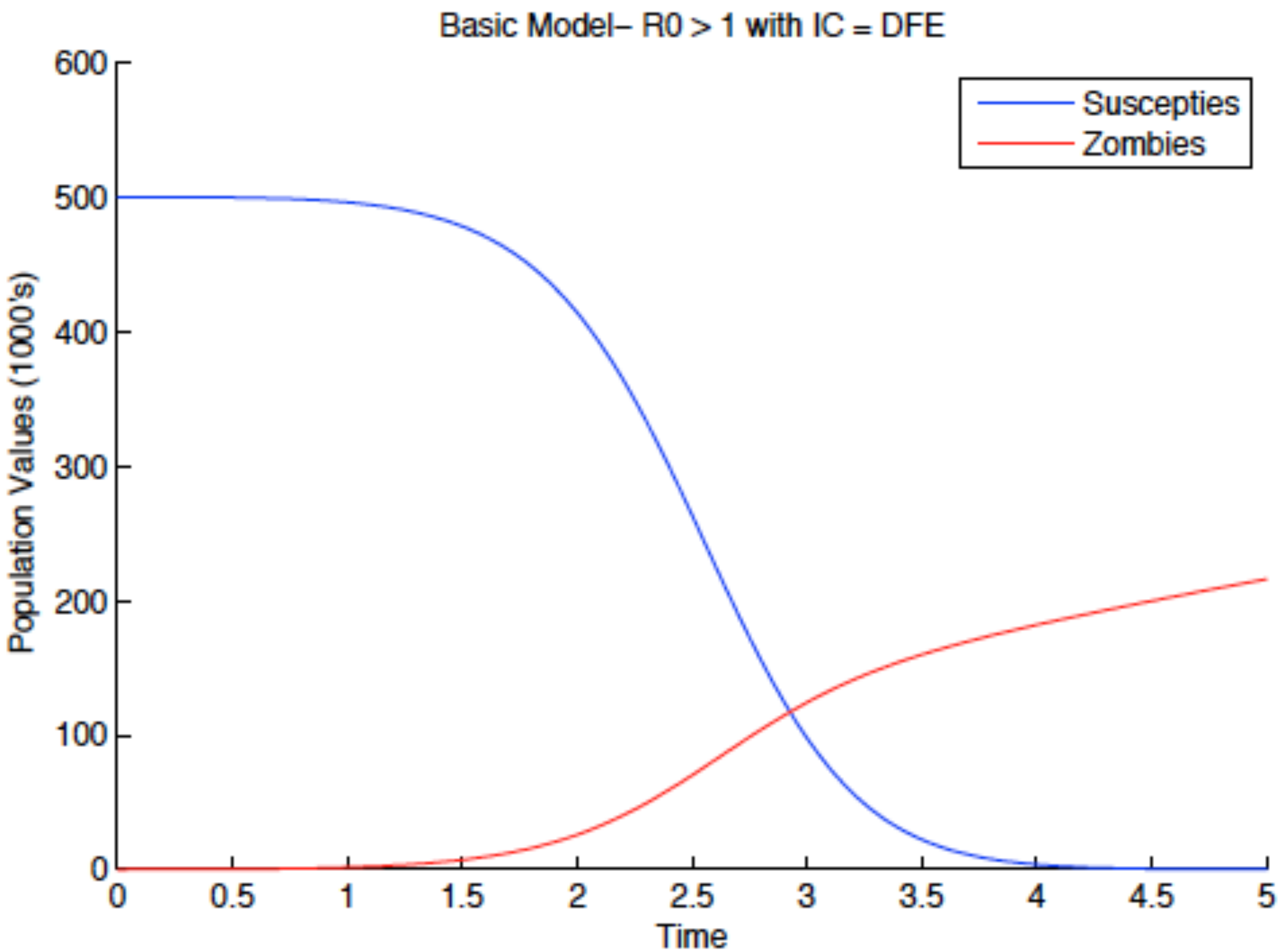
Computing with SZR

$$\begin{aligned} S' &= \Pi - \beta S Z - \delta S \\ Z' &= \beta S Z + \zeta R - \alpha S Z \\ R' &= \delta S + \alpha S Z - \zeta R\,. \end{aligned}$$

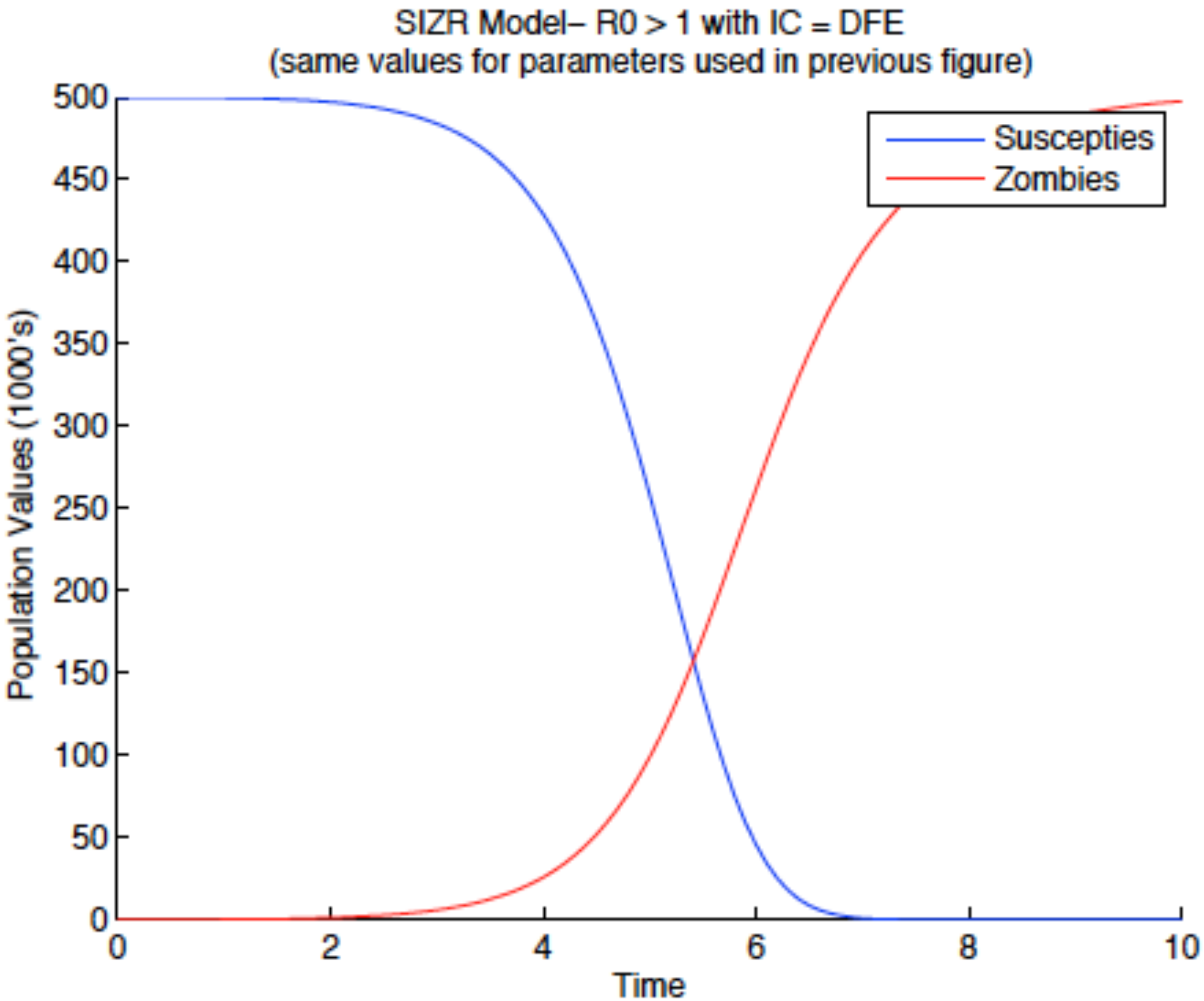
- Short timescale: (no births / natural deaths):

$$\begin{aligned} -\beta S Z &= 0 \\ \beta S Z + \zeta R - \alpha S Z &= 0 \\ \alpha S Z - \zeta R &= 0\,. \end{aligned}$$

Using Euler's Method



Model with Latent Infection

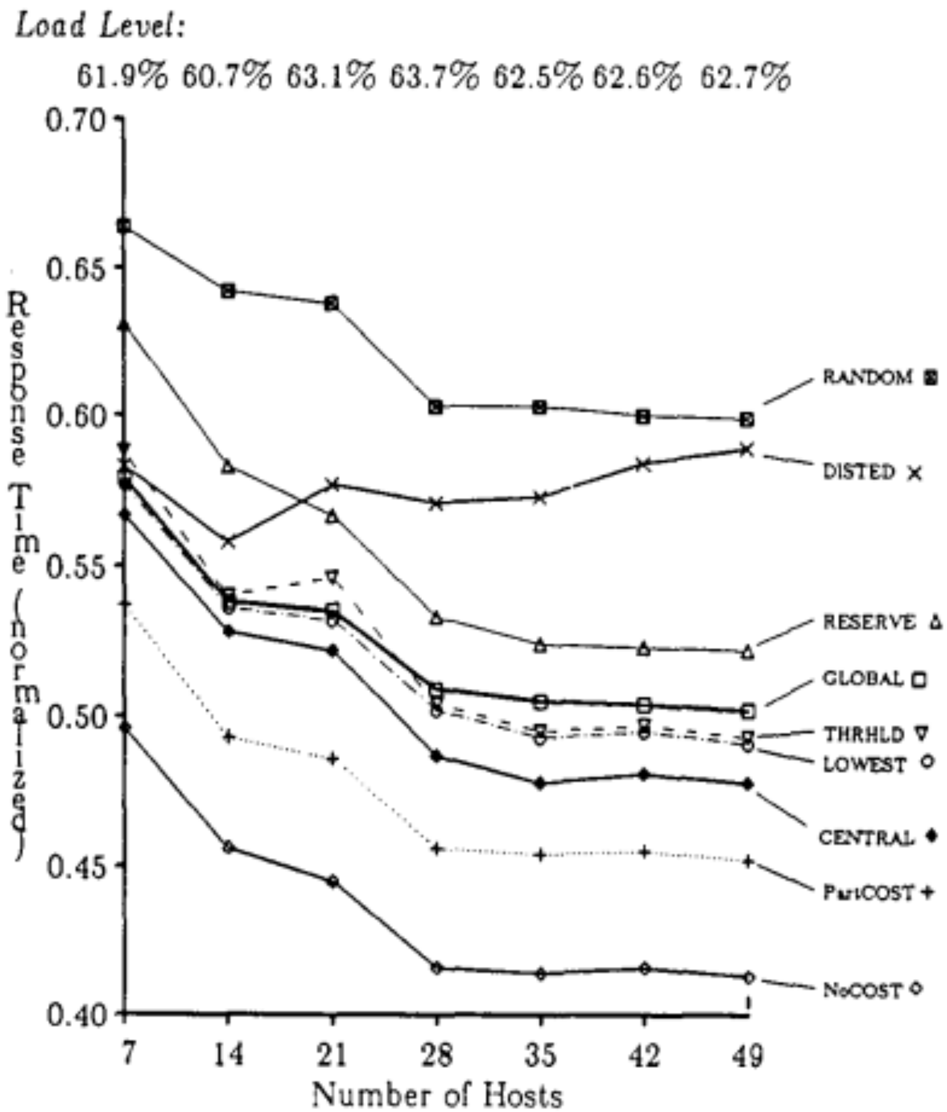


Alternative Zombie Sim

- http://kevan.org/proce55ing/zombies/

Event-Driven Examples

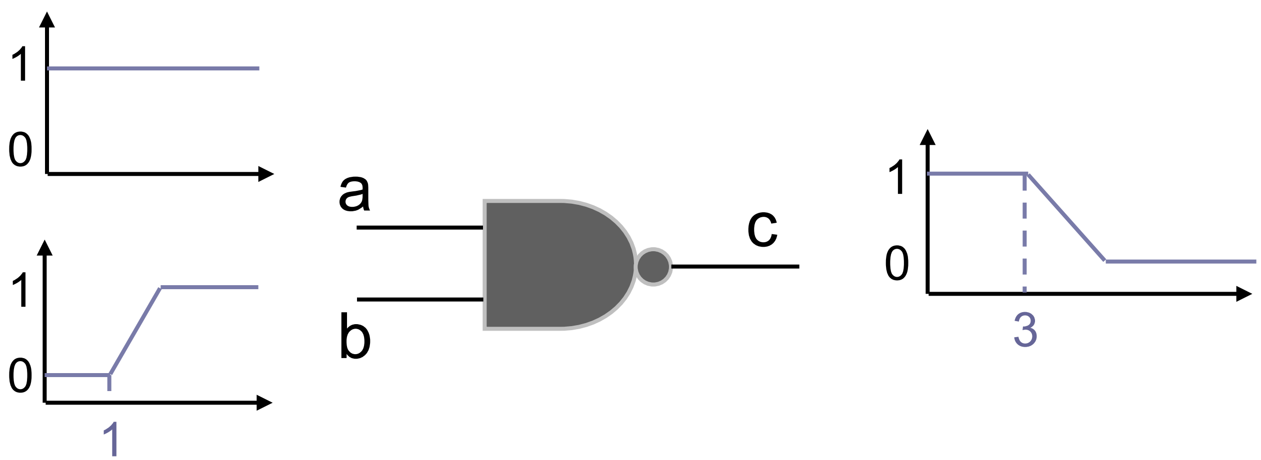
Example: Load Balancing Across Hosts



From Zhou, S. 1988. "A trace-driven simulation study of dynamic load balancing." *IEEE Trans. Software Eng.* 14(9).

Event-Driven Simulation

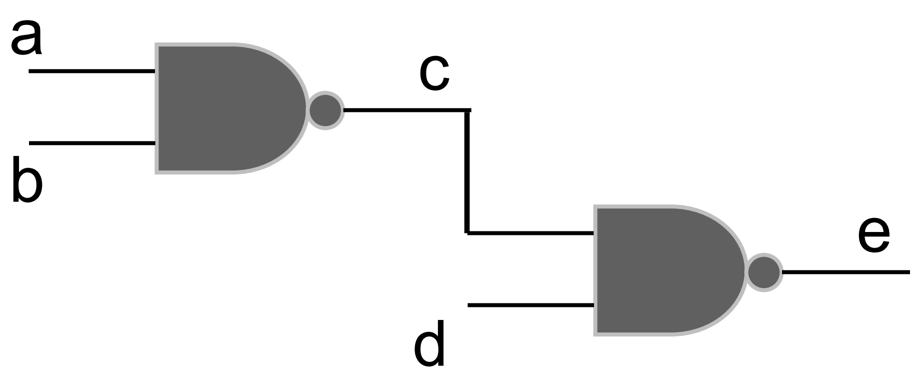
- Applications:
  - Circuit/chip simulation: clock rate needed for reliable operation



Events:
•Input: b(1)=1
•Output: c(3)=0

Event-Driven Simulation

- Applications:
  - Circuit/chip simulation: clock rate needed for reliable operation



Ingredients of Event-Driven Simulations

- Event queue
  - Holds (time, event) tuples
  - Priority queue data structure: supports fast query of event with lowest time
  - Possible implementation: linked list O(n) insertion, O(1) query, O(1) deletion
  - Possible implementation: heap, binary tree O(log n) insertion, O(1) query, O(log n) deletion

Ingredients of Event-Driven Simulations

- Event loop
  - Pull lowest-time event off event queue
  - Process event
    - Decode what type of event
    - Run appropriate code
    - (Compile statistics)
    - Insert any new events onto queue
  - Repeat.

Ingredients of Event-Driven Simulations

- How are new events scheduled?
  - Some are a direct result of current event.
    Example: teller takes new customer
  - Some are background events.
    Example: new customer arrives
  - Some are generated via real-time user input

Stochastic Simulation

- Events have different likelihoods of occurrence
  - New customer arrives
  - Person contracts disease
- Properties of simulation components may vary
  - Bank customers may have more or less difficult problems
  - Drivers may be more or less polite
  - Individuals may be more or less susceptible to disease

Sources of "Randomness"

- "Digital Chaos": Deterministic, complicated. Examples: pseudorandom RNGs in code, digital slot machines.
- "Analog Chaos": Unknown initial conditions. Examples: roulette wheel, dice, card shuffle, analog slot machines.
- "Truly random": Quantum mechanics. Examples: some computer hardware-based RNGs

“Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin.”

--- John von Neumann (1951)

Using RNGs

How would you…

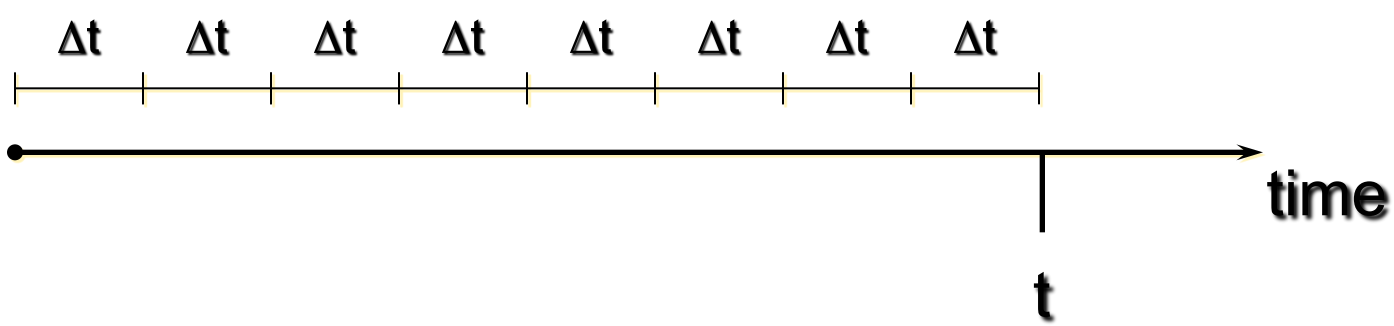
- Choose an integer *i* between 1 and *N* randomly
- Choose from a discrete probability distribution; example: *p(heads)* = 0.4, *p(tails)* = 0.6
- Pick a random point in 2-D: square, circle
- Shuffle a deck of cards

Bank Simulation: Scheduling Arrival Events

- Given time of last customer arrival, how to generate time of next arrival?
- Assume arrival rate is uniform over time: *k* customers per hour
- Then in any interval of length Δt, expected number of arrivals is $k\Delta t$

Scheduling Arrival Events

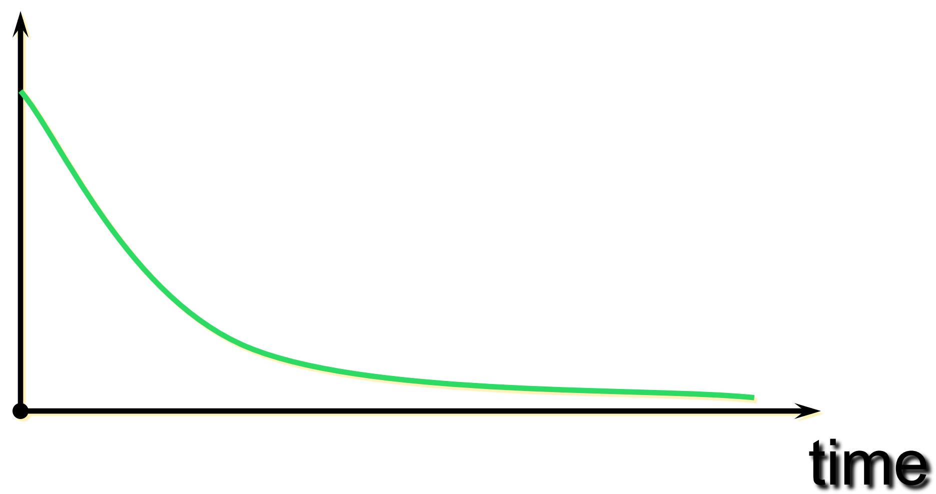
- Probability distribution for next arrival?
  - Equal to probability that there are no arrivals before time t
  - Subdivide into intervals of length Δt



p(no arrivals before t) = p(no arrival between 0 and Δt) *
p(no arrival between Δt and $2\Delta t$) * …

Scheduling Arrival Events

- p(no arrival in interval) = 1 – $k\,\Delta t$
- So, p(no arrivals before t) = $\lim_{\Delta t \to 0} \left(1 - k\,\Delta t\right)^{\frac{t}{\Delta t}} = e^{-kt}$

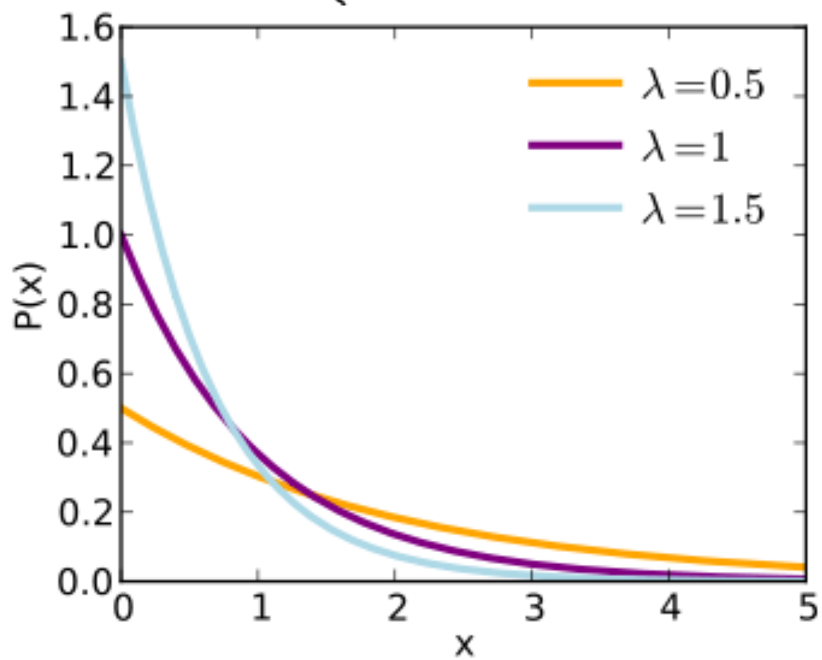


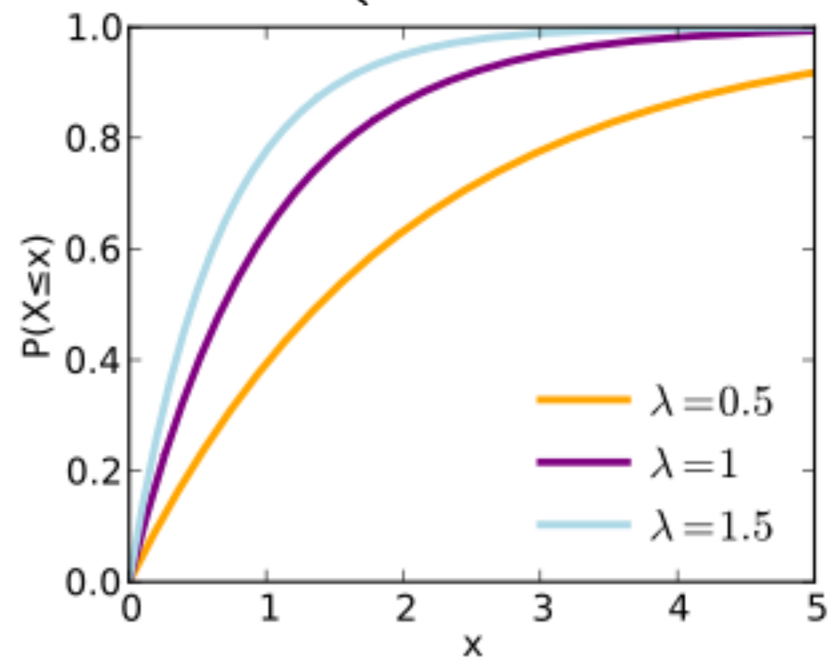
Exponential Distribution

- The exponential distribution describes the time in between events in a Poisson process

$$f(x;\lambda) = \begin{cases} \lambda e^{-\lambda x}, & x \geq 0, \\ 0, & x < 0. \end{cases}$$

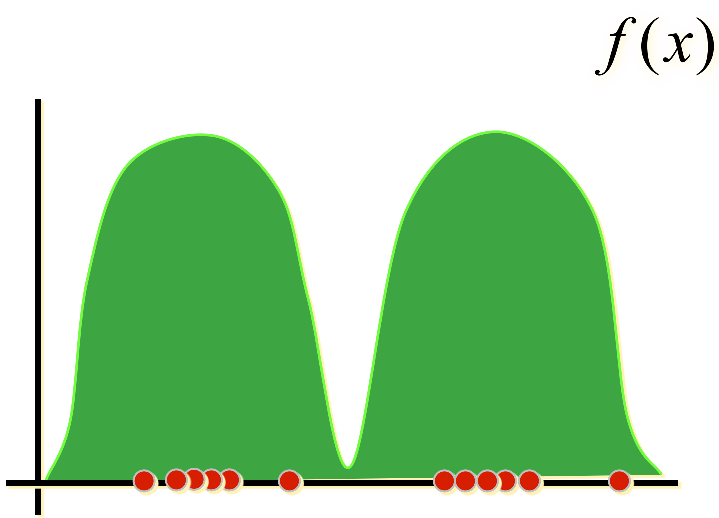
$$F(x;\lambda) = \begin{cases} 1 - e^{-\lambda x}, & x \geq 0, \\ 0, & x < 0. \end{cases}$$

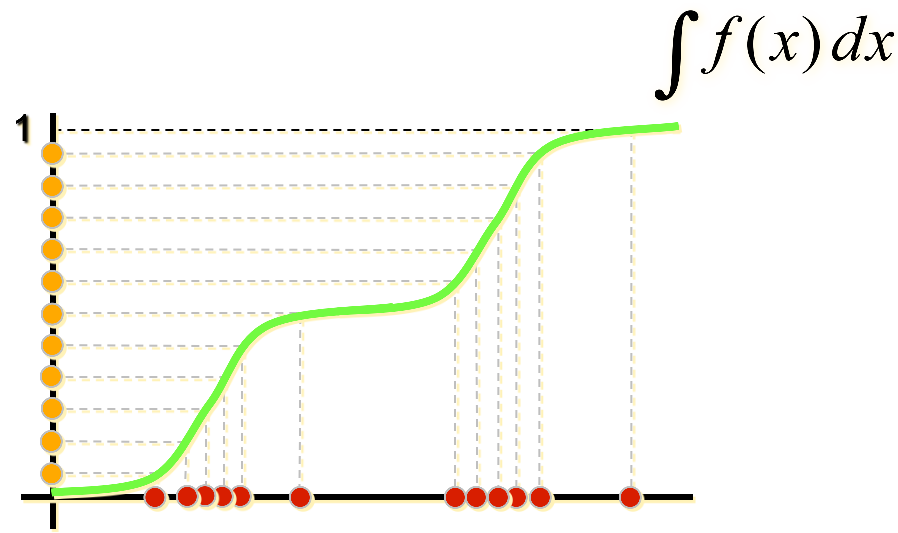




Sampling from a non-uniform distribution

- "Inversion method"
  - Integrate *f*(*x*): Cumulative Distribution Function
  - Invert CDF, apply to uniform random variable





Sampling from the Exponential Distribution

- time to next arrival event can be found from uniform random variable $\xi \in [0..1]$ via

$$t = -\frac{\ln \xi}{k}$$

Ingredients of Event-Driven Simulations

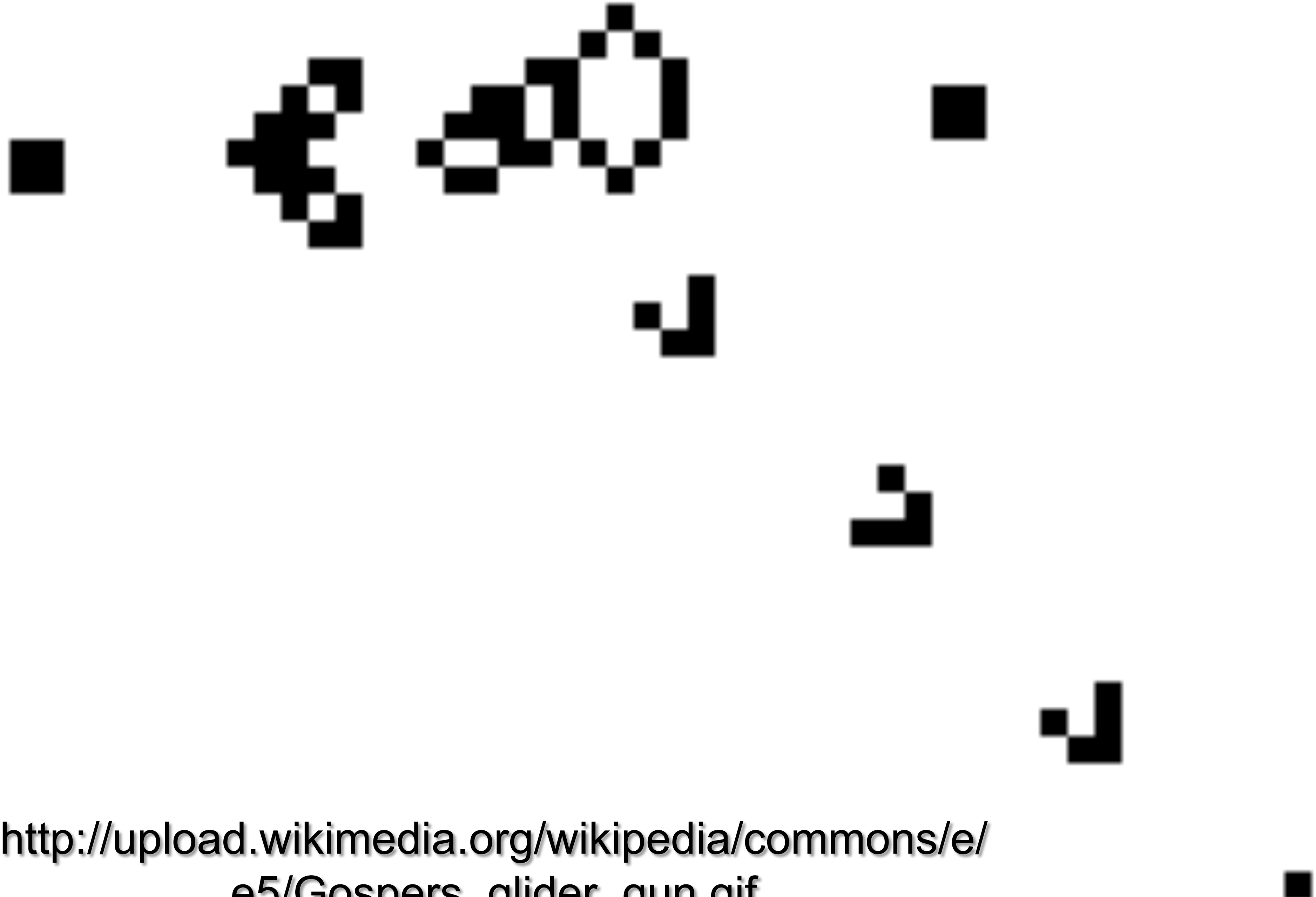
- How are events handled?
  - Need to run different piece of code depending on type of event
  - Code needs access to data: which teller? which customer?
  - Original motivation for Object-Oriented Programming languages: encapsulate data and code having a particular interface
  - First OO language: Simula 67

Summary

- Insert events onto queue
- Repeatedly pull them off head of queue
  - Decode
  - Process
  - Add new events

CAs, Microsimulation and Agent-based Simulation

(Micro-level behaviors leading to emergent macro-level phenomena)



http://upload.wikimedia.org/wikipedia/commons/e/e5/Gospers_glider_gun.gif

Cellular Automaton

- Discrete-time, discrete-space model
- Cells in grid have finite number of states
- Each cell's new state is a function of its previous state and the previous states of its neighbors
  - Typically instantaneous updates, same rules for all cells

Microsimulation

- Model components of system as independent entities with differing characteristics
  - e.g., different susceptibility to disease
- Behavior is governed by particular rules
- Useful in traffic, health, econometrics (e.g., taxation)
- Demo:
  - http://www.traffic-simulation.de/

Agent-Based Modeling

- Accommodates interdependencies, adaptive behaviors
- E.g., “The evolution of cooperation”

The Prisoner's Dilemma

Prisoner A's Strategies	Prisoner B's Strategies: Do Not Confess	Prisoner B's Strategies: Confess
Do Not Confess	1 Year / 1 Year	Parole / Life
Confess	Life / Parole	20 Years / 20 Years

- Globally optimal: Neither confesses
- Game-theoretically optimal strategy: Always confess

The Evolution of Cooperation

- Robert Axelrod: A tournament for simulations to play with each other in repeated rounds
- Winning strategy: TFT
- All top strategies are “nice”
- Necessary conditions for success:
  - Be nice
  - Be provocable
  - Don’t be envious
  - Don’t be too clever

A better strategy

- Jennings et al. in 2004 tournament:
  - Submit multiple prisoners and collude

Simulating Population Genetics

Simulating population genetics (assignment 5)

- review of basic genetics: genes, alleles
- If there are two possible alleles at one site, say A and a, there are in a diploid organism three possible genotypes: AA, aa, Aa, the first two homozygotes, the last heterozygote
- Question: How are these distributed in a population as functions of time?

Why study this?

- Understanding history of evolution, human migration, human diversity
- Understanding relationship between species
- Understanding propagation of genetic diseases
- Agriculture

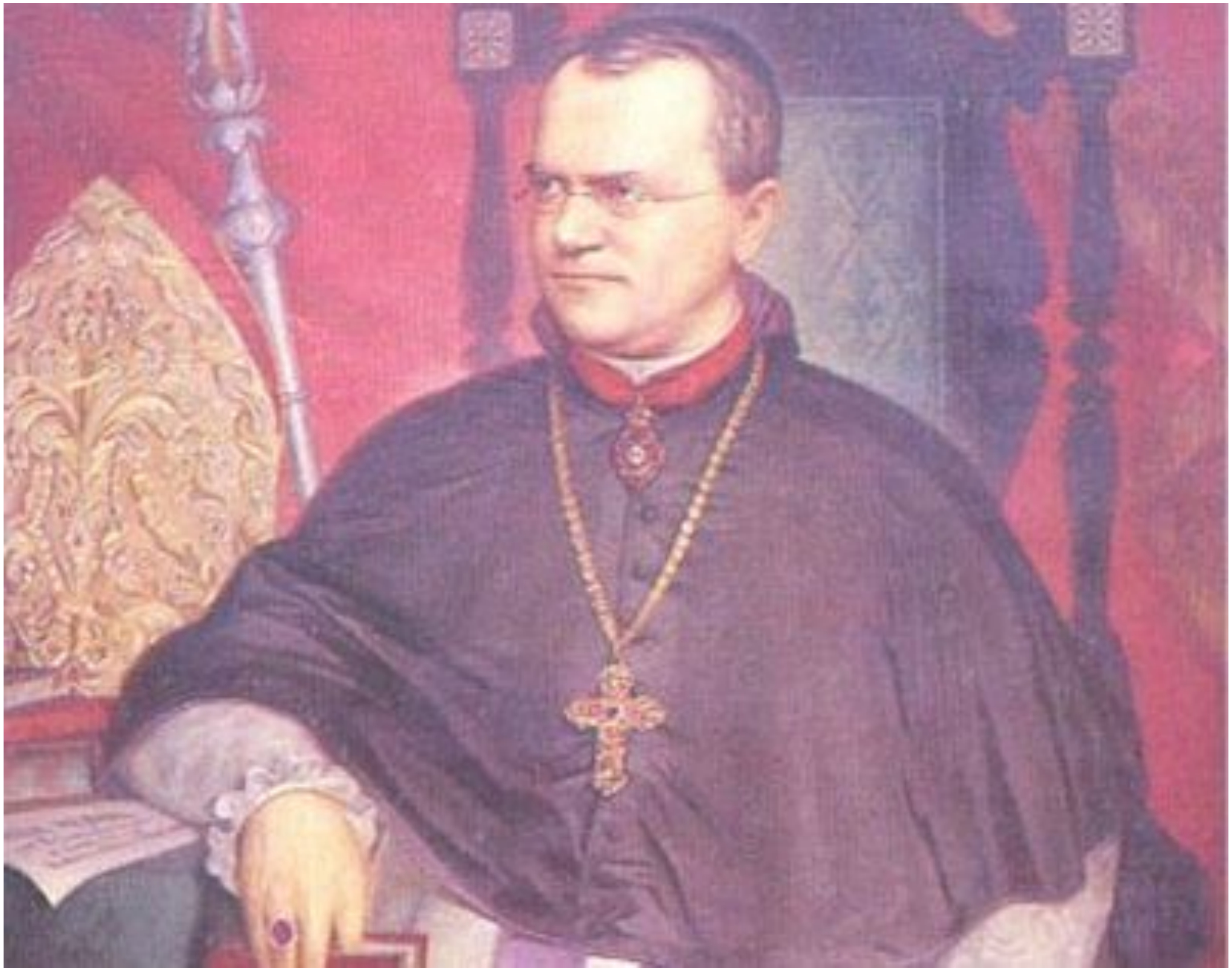
Approaches, pros and cons

- Field experiment
  + realistic
  - hard work for one particular situation
- Mathematical model
  + can yields lots of insight, intuition
  - usually uses very simplified models
  - not always tractable
- Simulation
  + very flexible
  + works when math doesn’t
  - not easy to make predictions

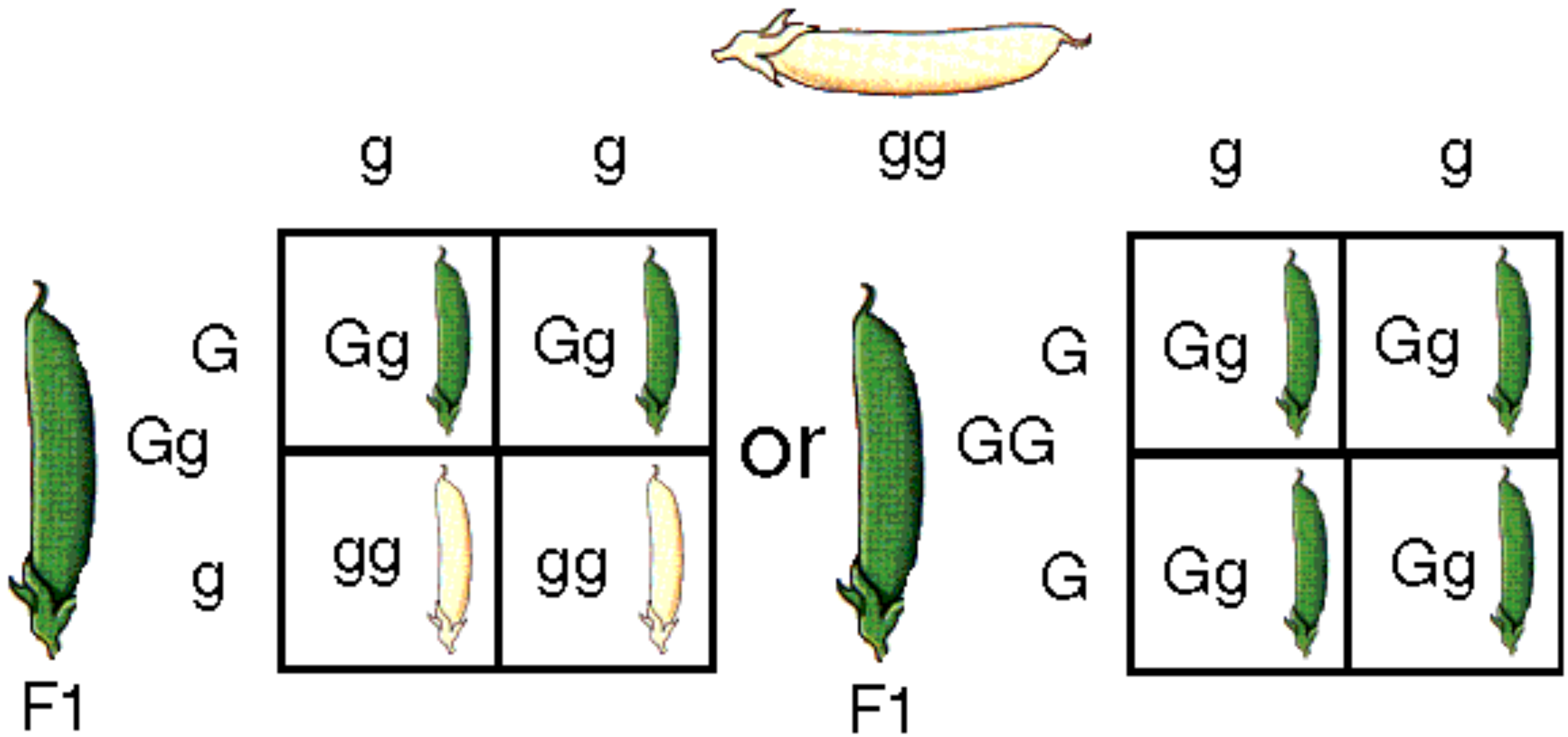
19th Century: Darwin et al. didn't know about genes, etc., and used the idea of *blended inheritance*

→But this requires an unreasonably large mutation rate to explain variation, evolution

Enter Mendel… (rediscovered in 20th century)



Gregor Mendel (1822 - 1884)



http://bio.winona.edu/berg/241f00/Lec-note/Mendel.htm

Steven Berg, Winona State

Simplest Model

- Hardy-Weinberg equilibrium
  - If probability of allele A is p, of a is q=1-p
    p(AA) = p^2, p(Aa) = 2pq, p(aa) = q^2
- Not always observed
  - Wahlund effect: fewer heterozygotes if multiple isolated subpopulations
  - Differences in viability, mating preference
- Assignment 5: limitations of theoretical model
  - Finite population, others