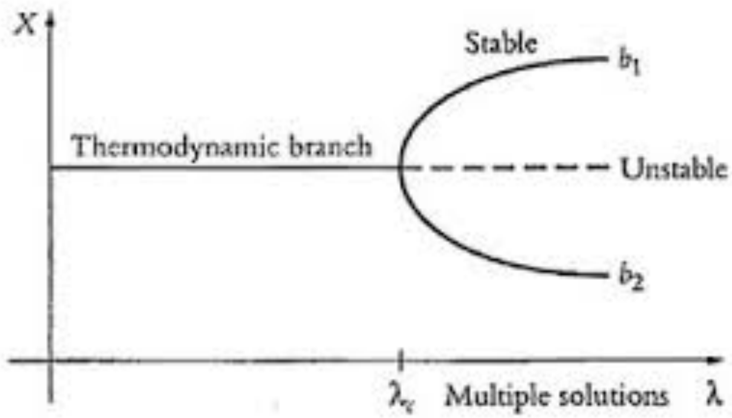
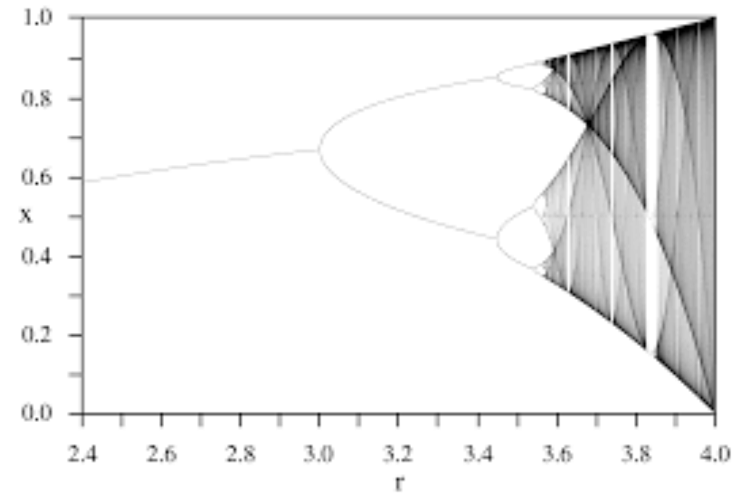
Complexity Science





$$\dot{x}_i = (1-\mu) f_i x_i + \mu \sum_{<j>_i} x_j - x_i \vec{\Phi}$$

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Outline

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Introduction: view on dynamics

Mean field models (ODEs)

- One dimensional systems (n=1)

  Fixed points and linear stability

  Bifurcations in one dimension: normal forms

- Two dimensional systems (n=2)

  Linear stability analysis: invariant objects in 2D

  Hopf-Andronov bifurcation

- Dynamics in n ≥ 3

  Global bifurcations. Chaos

Numerical methods

View on dynamics

History

Dynamics: interdisciplinary science (originally branch of physics)

Subject began in the mid-1600s

Newton (1643-1727):

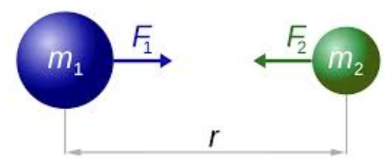
Invented differential equations

Discovery of the laws of motion and universal gravitation

Combined them to explain Kepler's law of planetary motion

Newton solved the two-body problem

(motion of the earth around the sun)



$$F_1 = F_2 = G\frac{m_1 \times m_2}{r^2}$$

Extension to the three-body problem (impossible analytically)

Poincaré (s. XIX-XX)

Qualitative dynamics

Powerful geometric approach

First to glimpse the possibility of chaos (deterministic systems with aperiodic behavior with dependence on i.cs.)

View on dynamics

Dynamics - A Capsule History

1666	Newton	Invention of calculus, explanation of planetary motion
1700s		Flowering of calculus and classical mechanics
1800s		Analytical studies of planetary motion
1890s	Poincaré	Geometric approach, nightmares of chaos
1920–1950		Nonlinear oscillators in physics and engineering, invention of radio, radar, laser
1920–1960	Birkhoff Kolmogorov Arnol'd Moser	Complex behavior in Hamiltonian mechanics
1963	Lorenz	Strange attractor in simple model of convection
1970s	Ruelle & Takens	Turbulence and chaos
	May	Chaos in logistic map
	Feigenbaum	Universality and renormalization, connection between chaos and phase transitions
		Experimental studies of chaos
	Winfree	Nonlinear oscillators in biology
	Mandelbrot	Fractals
1980s		Widespread interest in chaos, fractals, oscillators, and their applications

Dynamical systems (DS)

Iterated maps (difference eqs.): evolution of systems in discrete time

Differential equations: evolution of systems in continuous time

Differential equations:

ODEs

$$m\frac{d^2x}{dt^2}+b\frac{dx}{dt}+kx=0$$

Ordinary derivatives: dx/dt and d^2x/dt^2

Only 1 independent variable (time t)

and

PDEs

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}$$

2 independent variables (time t, space x)

ODEs

$$\begin{aligned}\dot{x}_1 &= f_1(x_1, \ldots, x_n)\\ &\vdots\\ \dot{x}_n &= f_n(x_1, \ldots, x_n).\end{aligned}$$

Here the overdots denote differentiation with respect to t. Thus $\dot{x}_i \equiv dx_i/dt$. The variables $x_1, \ldots, x_n$ might represent concentrations of chemicals in a reactor, populations of different species in an ecosystem, or the positions and velocities of the planets in the solar system. The functions $f_1, \ldots, f_n$ are determined by the problem at hand.

For example, the damped oscillator (1) can be rewritten in the form of (2), thanks to the following trick: we introduce new variables $x_1 = x$ and $x_2 = \dot{x}$. Then $\dot{x}_1 = x_2$, from the definitions, and

$$\begin{aligned}\dot{x}_2 = \ddot{x} &= -\tfrac{b}{m}\dot{x} - \tfrac{k}{m}x\\ &= -\tfrac{b}{m}x_2 - \tfrac{k}{m}x_1\end{aligned}$$

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = 0$$

from the definitions and the governing equation (1). Hence the equivalent system (2) is

$$\begin{aligned}\dot{x}_1 &= \boxed{x_2}\\ \dot{x}_2 &= \boxed{-\tfrac{b}{m}x_2 - \tfrac{k}{m}x_1.}\end{aligned}$$

Linear: variables at the right to the first power

Types of dynamical systems

ODEs: Deterministic vs stochastic (Langevin eqs, Gillespie)

Time continuous, no space, continuous state variables,

finite dimension (= number of state variables)

1D – fixed points

2D – oscillations (limit cycles, centers)

3D – periodic orbits, chaos -> d > 3, high-dimensionalsystems

PDEs: Deterministic vs stochastic

Time and space continuous, continuous state variables,

infinite dimension (discretization to solve)

DDEs: Deterministic vs stochastic

Time continuous, no space, continuous state variables, infinite dimension

- Continuous delay

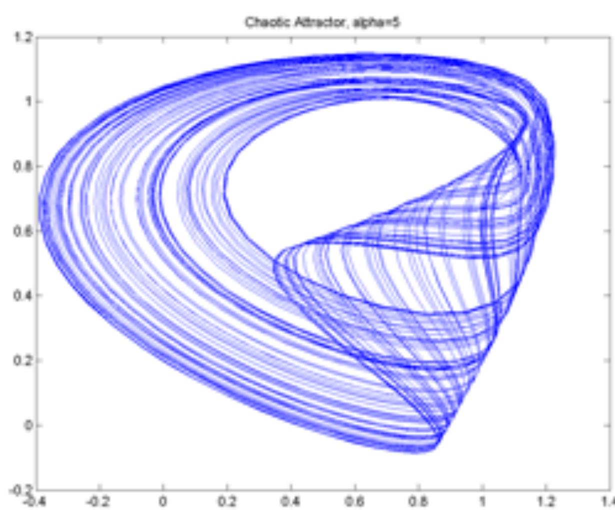
$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = f\left(t, x(t), \int_{-\infty}^{0} x(t+\tau)\,\mathrm{d}\mu(\tau)\right)$$

$$\frac{dx}{dt} = \beta \frac{x_\tau}{1 + {x_\tau}^n} - \gamma x,$$

$$\gamma, \beta, n > 0,$$

- Discrete delay

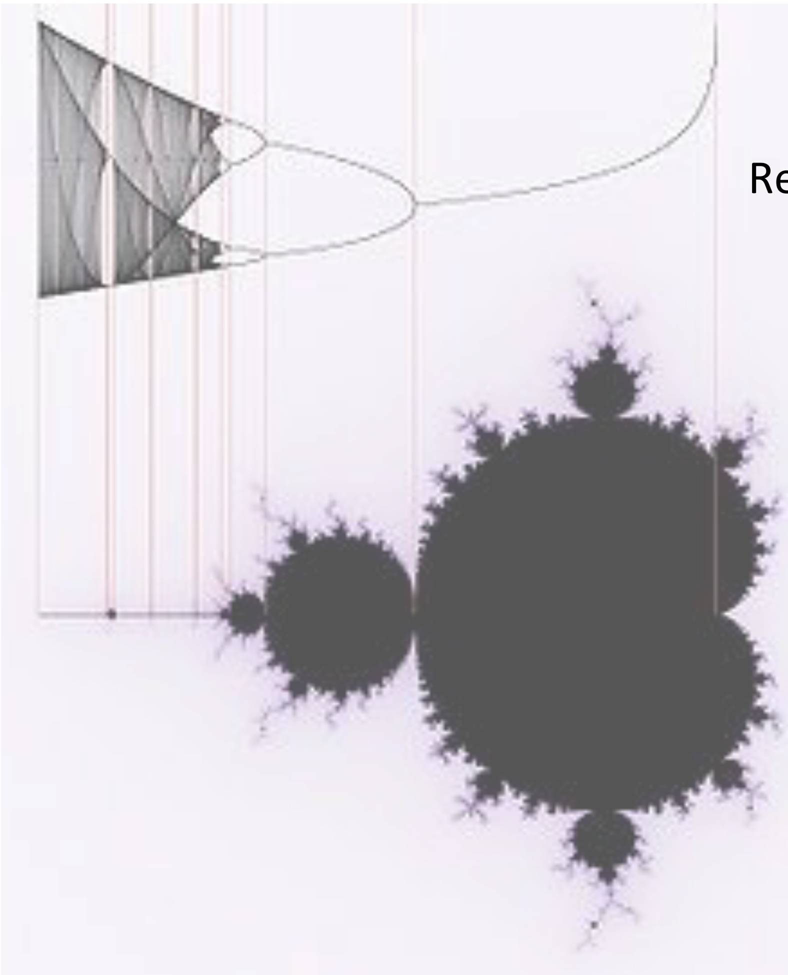
$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = f(t, x(t), x(t-\tau_1), \dots, x(t-\tau_m)) \text{ for } \tau_1 > \dots > \tau_m \geq 0.$$



Types of dynamical systems

IMs: Deterministic vs stochastic

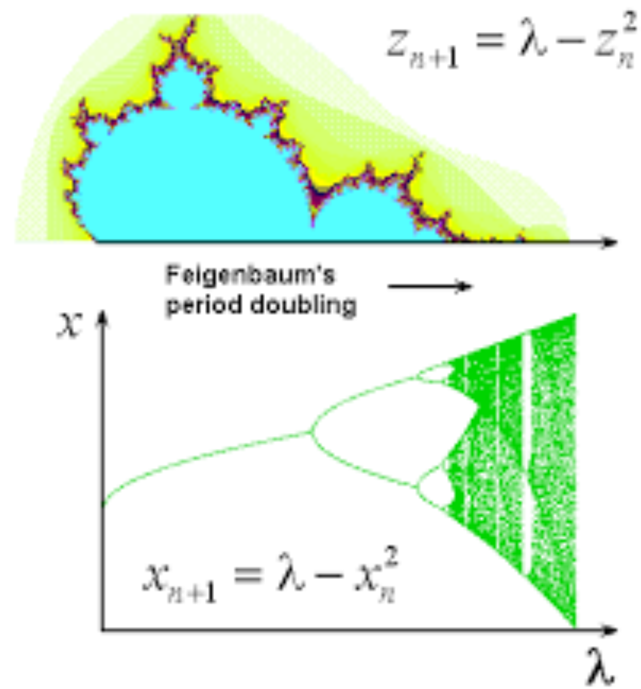
Time discrete, finite dimension



$$x_{n+1} = r x_n (1 - x_n)$$

Real numbers

Complex numbers



Types of dynamical systems

Agent-based models: Deterministic vs stochastic (MonteCarlo simulations)

Time discrete, discrete state variables

MonteCarlo methods

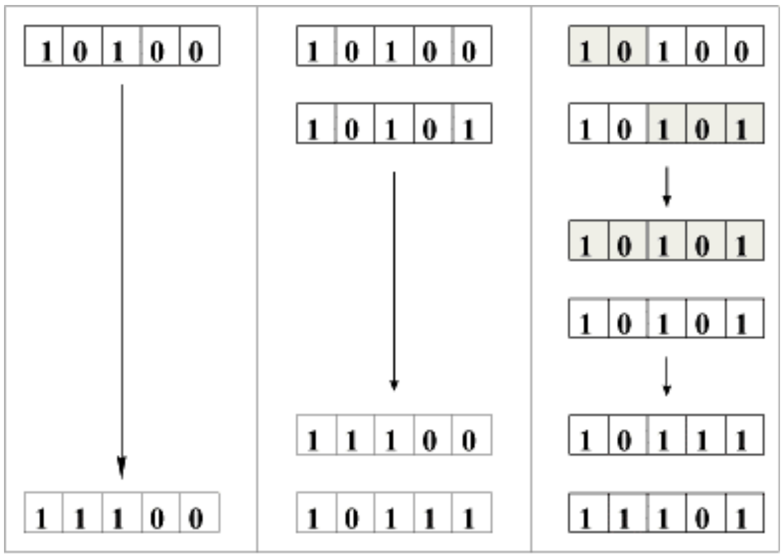
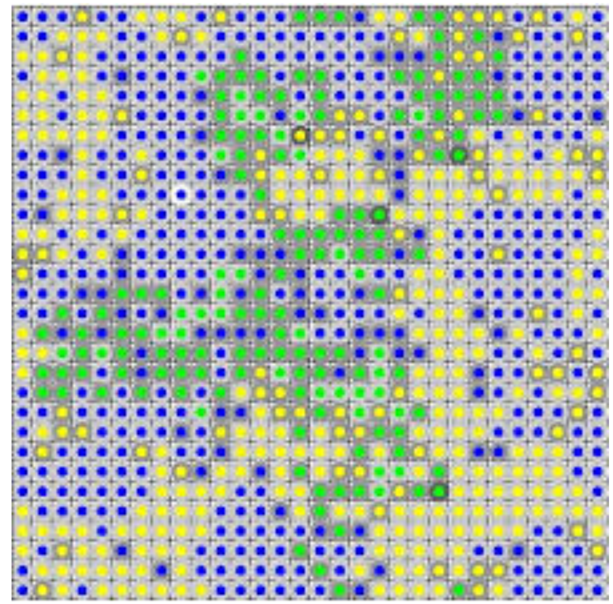


Fig. 2a – Schematic representation of the genomic changes for AS, AP, MP (from left to right).

Bit-string models
Gillespie Method
Tau-leap method

Cellular automata models



We can convert them to mean field models to study their deterministic dynamics and qualitative features (bifurcations, etc etc). Breaking spatial correlations

Discrete state-variables, time, and space

State space: 1D, 2D, 3D lattice

States of the CA (agent-based model): individuals, types of tumor celss, …

State-transition rules: replication, mutation, diffusion, …

Neighborhood: 4 nearest cells, 8 nearest cells, …

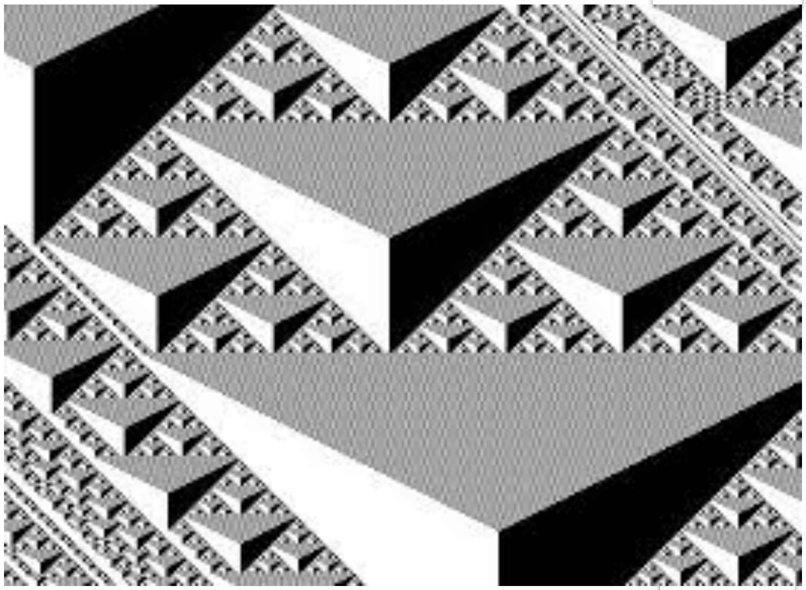
Boundary conditions: periodic, zero-flux, …

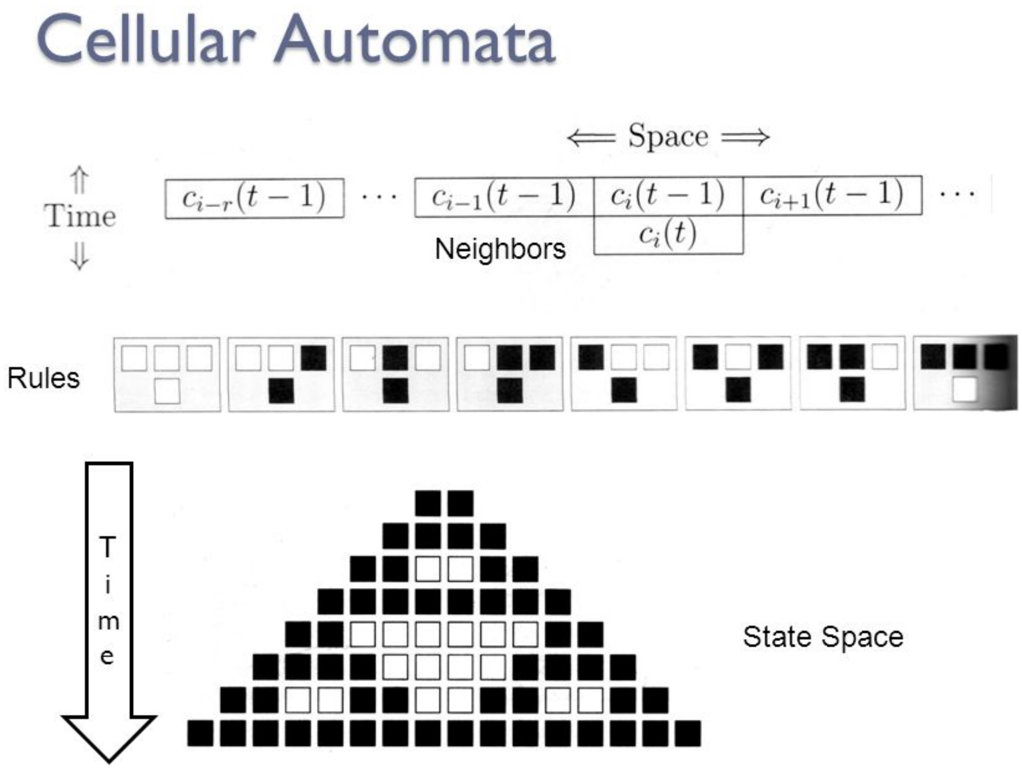
Types of Cas

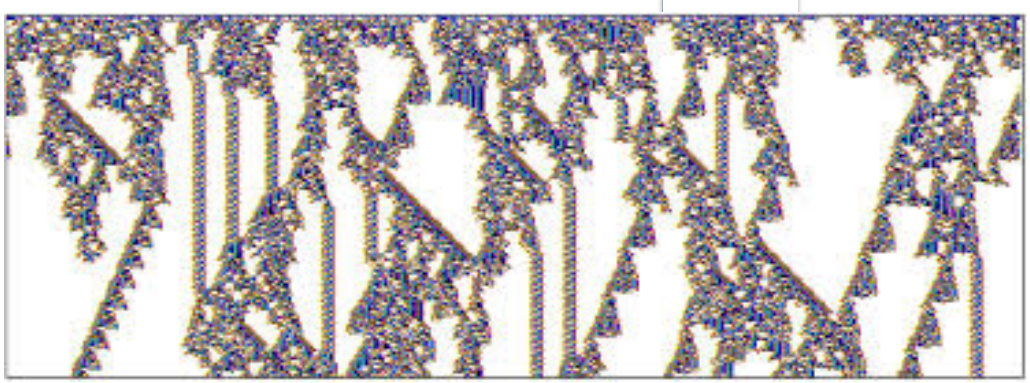
Deterministic vs stochastic
Synchronous vs asynchronous

If we break spatial correlations in a CA and use large lattice sizes, the dynamics is usually equivalent to the mean field approach

State space: One-dimensional



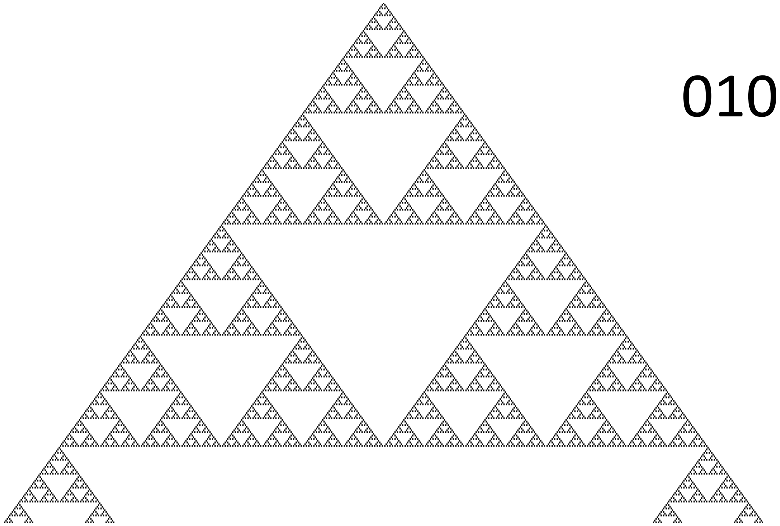




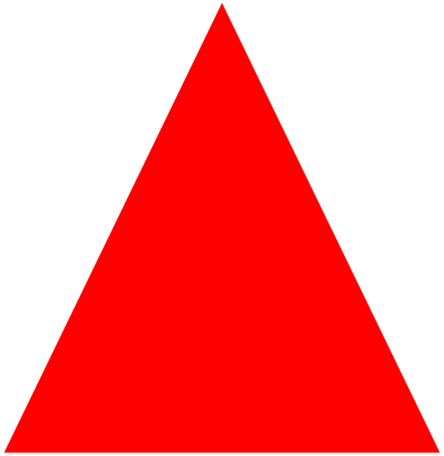
State space: One-dimensional (elementary CA)

In the case of Rule 90 , each cell's new value is the exclusive or of the two neighboring values. Equivalently, the next state of this particular automaton is governed by the following rule table:

current pattern	111	110	101	100	011	010	001	000
new state for center cell	0	1	0	1	1	0	1	0



$$01011010_2 = 90_{10}$$



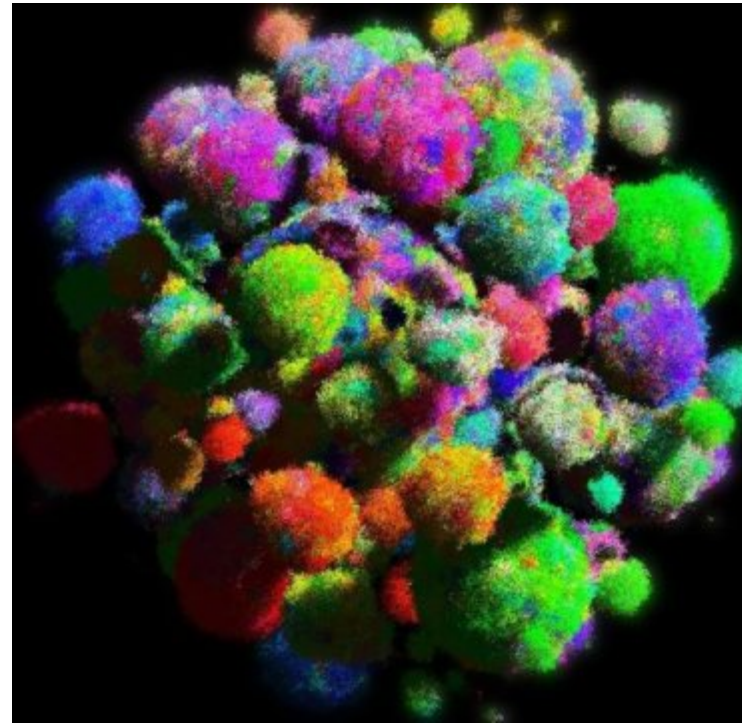
Sierpinski triangle

Spatial cancer simulations

Many cancers are large (cms in diameter)
Billions of cells
Evidences that mutations emerge late during tumor progression

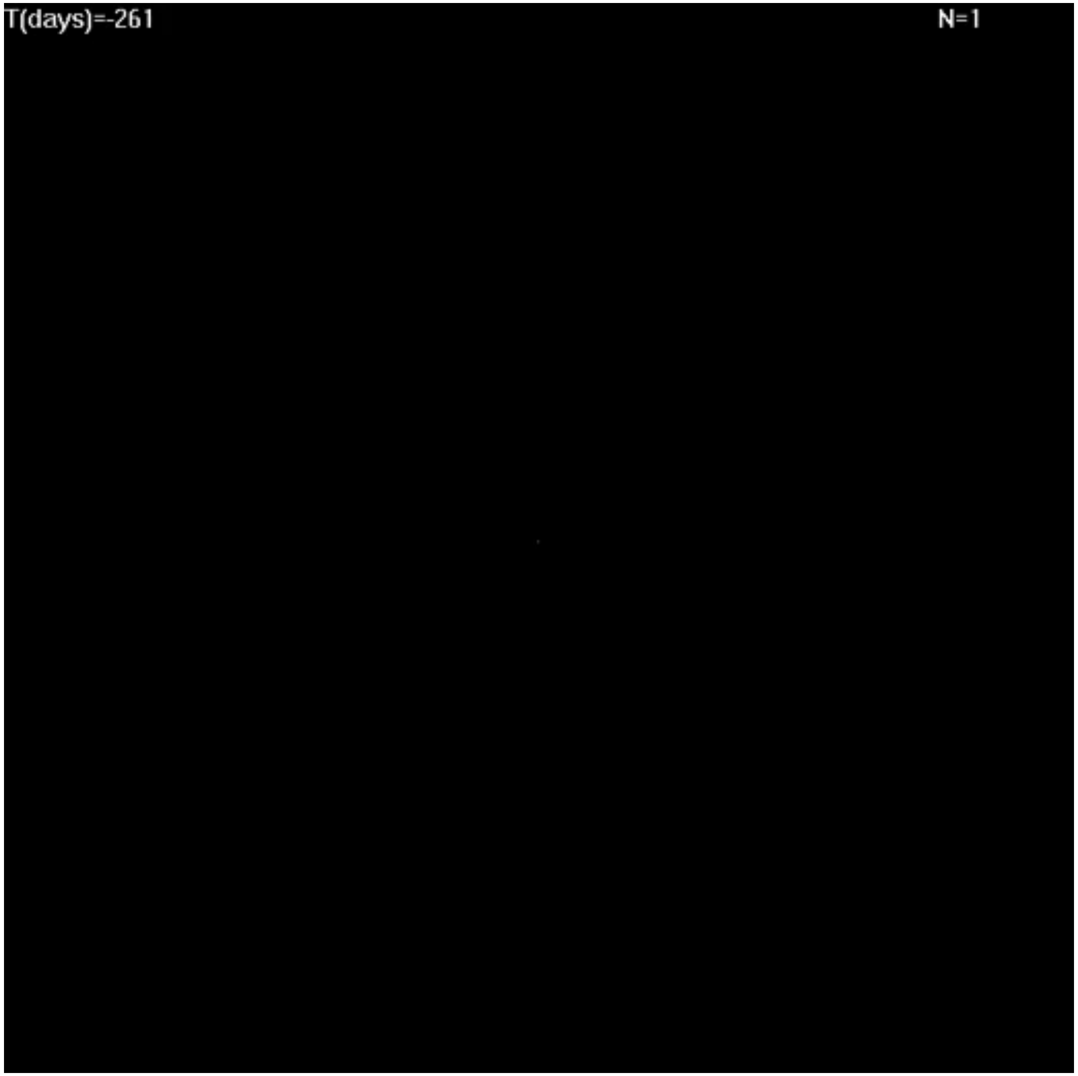
Questions to answer with the model:
How such alterations expand within a 3D spatial tissue, and come to dominate a large, pre-existing lesion

Model with : short-range dispersal and cell turnover



Waclaw et al. Nature 252: 261-264 (2015)

Animation of tumor growth (plus treatment and tumor relapse)



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Dimensions and dynamics

n = 1	n = 2	$n \geq 3$	$n \gg 1$	$n = \infty$
Growth and decay	*Oscillations*	*Chaos*	*Collective phenomena*	*Waves and patterns*
Fixed points	Pendulum	Strange attractors (Lorenz)	Josephson arrays	Solitons
Bifurcations	Anharmonic oscillators	Chemical kinetics	Coupled nonlinear oscillators	Plasmas
Overdamped systems	Limit cycles	3-body problem (Poincaré)	Iterated maps	Quantum field theory
Relaxational dynamics	Heart cells	Fractals (Mandelbrot)	Lasers	Earthquakes
Logistic model (single species)	Neurons	Simple Matching allele dynamics	Immune system	General relativity
Autocatalytic replicator	Nonlinear electronics	Quantum chaos?	“Advanced” hypercycles?	Turbulent fluids
Metapopulations (Levins)	Simple quasispecies (Eigen)	“Large” hypercycles?	Artificial protocell?	Reaction-diffusion
Chemical equilibrium	“Initial” hypercycles?	Trophic food chains	Ecosystems	Epilepsy
Catastrophes	Two-patch metapopulations	Red Queen dynamics	Economics	Protocell replication?
Symmetry breaking	Predator-prey systems		Origin of life?	Ecosystems
				Life

Table 1.1: Classification of several nonlinear systems according to the number of state variables (i.e., dimensions), n, of the ordinary differential equations describing their dynamics. The dynamical behaviors described in italics in the second row correspond to the more complex dynamics found in each dimension. Generically, such behaviors are additive as we move from left to right. That is, for example, the case $n \geq 3$ can also behave like cases $n = 2$ or $n = 1$, but not the other way around (modified from [165]).