Introduction to Complex Systems II

Esteban Velez Ramirez

2016/02/08

Overview

1. Introduction

2. Ant Colony System

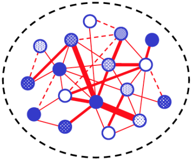
3. Irreversible Sytems: heat flux in a nonlinear chain

4. Relevance of computational modeling in complex system science

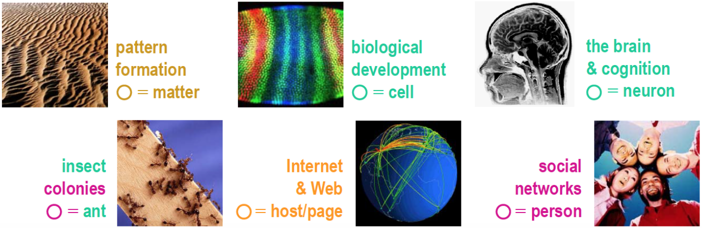
5. References

Introduction

What are complex systems?



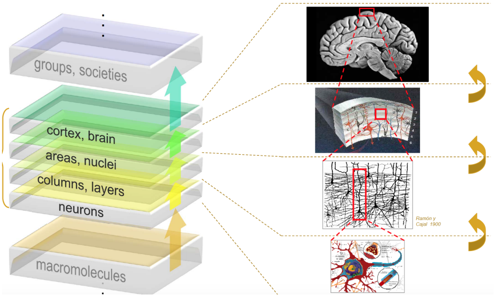
- Large number of agents interacting locally
- Complex emergent, self-organized behavior
- decentralized dynamics architect



Ant colony system

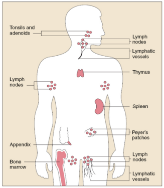
- The colony as a whole can work together cooperatively to accomplish very complex tasks.
- No central control
- They organize themselves to produce structures much more complicated than any single ant could produce

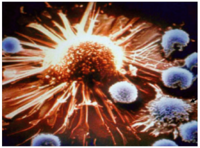
The brain



- 100 billion neurons and 100 trillion connections between those neurons.
- Somehow the huge ensemble of neurons and connections gives rise to the complex behaviors we call "cognition" or "intelligence" or even "creativity".

Immune system





- They communicate with one another through chemical signals, and work together, without any central control, to launch coordinated attacks on what they perceive as threats to the body.
- They are able to change, or adapt itself, in response to what that population of cells perceives in its environment

Cities

- It has often been said a city is like a living organism in many ways
- To what extent do cities actually resemble living organisms, in the ways they are structured, grow, scale with size, and operate?

Properties

Emergence

- The system has properties that the elements do not have
- These properties can not be easily inferred or deduced
- Different properties can emerge from the same elements

Self-organization

- “Order” of the system increases without external intervention
- Originates purely from interactions among the agents

Properties

Nonlinear interactions

- The components of the system interact in such a way that the overall behavior can not be expressed as the sum of the individual parts.

Information processing

- The system as hole gets information from the environment about its current state
- It uses this information to take decisions.

Properties

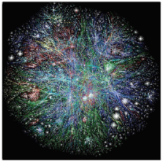
Evolution, adaptation and learning

- Systems improve by themselves in order to survive or have a better performance in its environment.

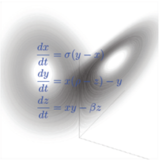
Decentralization

- The "invisible hand": order without a leader
- Distribution: each agent carry a small piece of the global information
- Ignorance: agents don’t have explicit group-level knowledge/goals

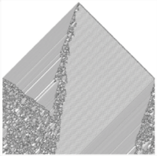
A vast archipielago



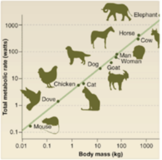
Complex networks



Dynamical systems

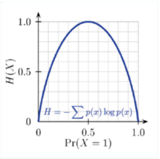


Cellular automata

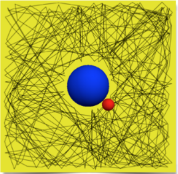


Scaling and criticality

Evolution, adaptation and game theory



Information theory



Statistical physics

Agent based modeling

Ant Colony System

Motivation

- Study self-organization
  - Modeled ⟶ Agent base modeling (ABM)
  - Theoretical framework ⟶ Nonequilibrium thermodynamics

Question

Is there a link between nonequlibrium thermodynamics and (AMB)?

System to study

- Ant colony food foraging
- Exhibit self-organization
- Can be modeled using ABM

The agents (the ants) $\longrightarrow$ Decisions $\longrightarrow$ Simple rules

Rules $\longrightarrow$ gradient-following and pheromone dropping

$$\Downarrow$$

Construct the shortest paths to food sources

Borrowing nonequilibrium thermodynamics ideas

1. Constraints can be constructed from entropy-producing processes in the bootstrapping phase of self-organizing systems.
2. Positive feedback loops are critical in the structure formation phase.
3. Constraints tend to decay. The continued presence of far-from-equilibrium boundary conditions are required to reinforce constraints in the maintenance phase.

Constraint

What is a constraint in the ant colony system?

As a system self-organizes, components of the system are expected to lose degrees of freedom.

↓

In the ant colony system, ants lose directional degrees of freedom as they are informed by a gradient. This is called a constraint.

↓

Quantities that measure ignorance and order

Entropy

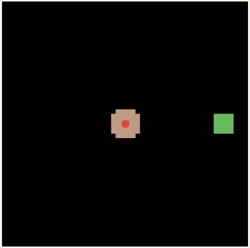
$$S = -\sum_{i=1}^{W} p_i \log p_i. \quad (1)$$

Model

- A nest and some amount of food are placed in the space
- A fixed number of ants is initially placed at the nest

↓

Initial configuration



Evolution

```
...: if ant has food then
...:        drop one unit of food pheromone
...:        if at nest then
...:              drop food
...:        else
...:              follow nest pheromones
...:        end if
...: else
...:        if not at food
...:               follow food pheromones
...:        else
...:               pick up food
...:        end if
...: end if
```

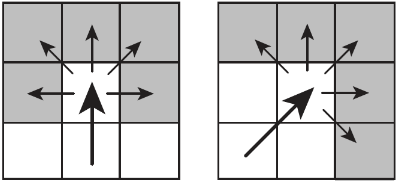
- At each time step some percentage of the pheromone present at each position evaporates

$$\Downarrow$$

Allows adaptation to changes in food location

- The ants have directionality. They can only travel to their forward five positions

$$\Downarrow$$



Borrowing ideas from Ant-Colony-Optimization (ACO)

$$p_j = \frac{\mu_j^\alpha + \beta}{\sum_{n-1}^{N} \mu_n^\alpha + \beta} \quad (2)$$

α: Scaling exponent

Increases the probability to the greatest pheromone level

β: Random base

Decrease the probability to the greatest pheromone level

μ_j

Pheromone level at position j

Directional entropy → Total ant ignorance

$$S_q = \frac{\sum_{i=1}^{N} p_i \ln p_i}{\ln N}, \tag{3}$$

Spatial entropy

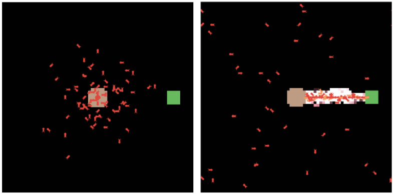
$$S_q = \frac{\sum_{i=1}^{M} \rho_i \ln \rho_i}{\ln M}, \tag{4}$$

where ρ is given by

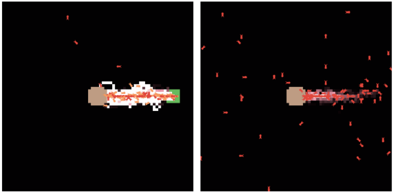
$$\rho_i = \frac{\text{\# of ants at position } j}{M}. \tag{5}$$

$$M \longrightarrow \text{Total number of positions in the space} \tag{6}$$

Evolution

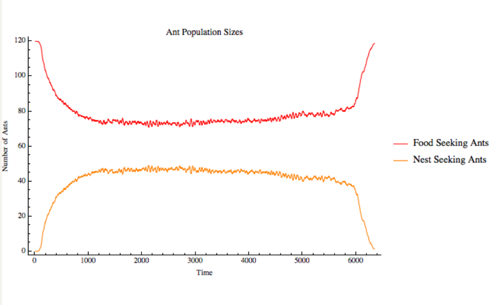


(a) Bootstrapping (b) Structure formation



(c) Structure maintenance (d) Re-exploration

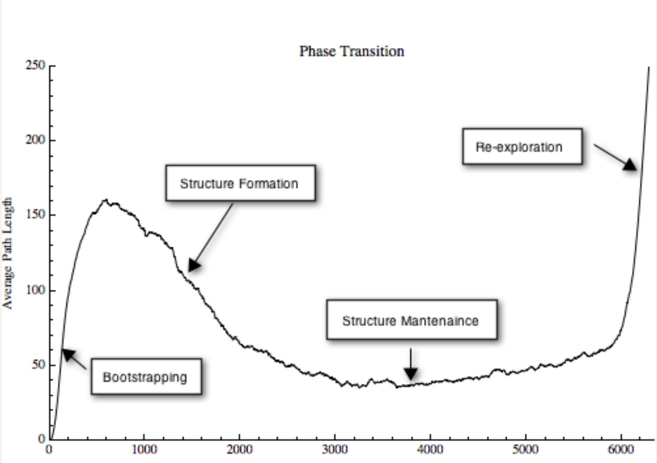
Population Sizes



- Population sizes of nest seeking and food seeking ants. Both populations achieve equilibrium once a path between the nest and the source of food is created.

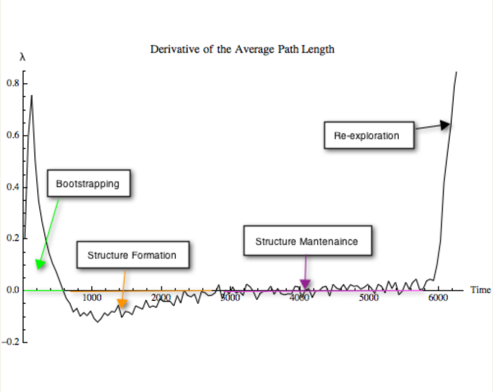
Different phases of evolution

Mean path length



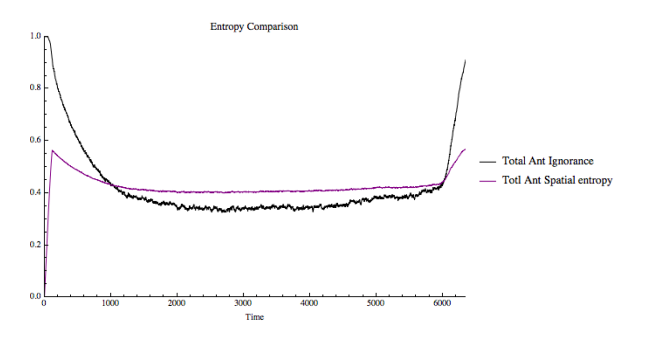
Different phases of evolution

Order parameter: $\lambda = \frac{d}{dt}$(Mean Path Length)



Measuring nonequilibrium thermodynamic properties

Entropy comparison



○ Increasing spatial entropy causally constraining ant movement is offered as an illustration of:

(1). Constraints can be constructed from entropy-producing processes in the bootstrapping phase of self-organizing systems.

○ When the food source is close to zero, the structure breaks up as the constraints on the ants movements (the pheromone field) gradually decay. This is an illustration of:

(3). Constraints tend to decay. The continued presence of far-from-equilibrium boundary conditions are required to reinforce constraints in the maintenance phase

Irreversible Sytems: heat flux in a nonlinear chain

Motivation

Irreversibility paradox

All the fundamental differential equations of physics — Einsten's, Hamiltons's, Lagrange's, Maxwell's, Newton's, Shrödinger— are "time reversible"

$\Downarrow$

THERMODYNAMICS AND EVERY DAY LIFE ARE NOT.

Introduction

Time reversibility

All possible solutions of the fundamental equations can be followed either forward or backward in time.

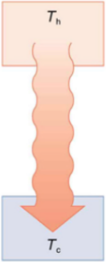
Computational roundoff errors accumulate.

No simple relation linking the errors in a reverse trajectory to those of the forward trajectory

$$\Downarrow$$

The exponential growth of these differences frustrate attempts to reverse trajectories for more than a few collision times

Irreversible flows



- impose boundary conditions or constraints
- Heat and work should be incorporated into the programing.

how this could be done ?

Thermal environment

Thermostats

A modification of the Newtonian MD scheme with the purpose of generating a statistical ensemble at constant temperature. It constrain the kinetic energy of selected degrees of freedom

$$\Downarrow$$

- Match experimental conditions
- Manipulate temperatures in algorithms
- Avoid energy drifts caused by accumulation of numerical errors

Temperature

Thermodynamics

Two bodies in thermal equilibrium with a third are also in thermal equilibrium with each other. This macroscopic thermodynamic ignores fluctuations

Statistical mechanics

Temperature T is defined by the average kinetic energy of any typical Cartesian degrees of freedom, relative to a commoving corotating frame

$$T = \frac{\langle p^2 \rangle}{mk}$$

- Kinetic-theory temperature can be used both at and away from equilibrium. At equilibrium, where entropy is a valid concept, the maximization of entropy invariably leads to the Maxwell–Boltzmann “Gaussian” distribution of momenta:

$$P(p) = \sqrt{\frac{\beta}{2\pi m}} e^{-\beta \frac{p^2}{2m}} \tag{7}$$

Molecular Dynamics Simulation

- Phase space is collection of positions q and momenta p of particles in system
- The Hamiltonian form

$$dq_t = \nabla_p H(q_t, p_t)dt \tag{8}$$

$$dp_t = -\nabla_q H(q_t, p_t)dt \tag{9}$$

$$H(q, p) = E_{kin} + V(q), \qquad E_{kin} = \frac{1}{2}p^T M^{-1} p \tag{10}$$

Nose-Hoover deterministic thermostat

- Based on extended Lagrangian formalism
  - Deterministic trajectory
  - Simulated system contains virtual variables related to real variables

$$\dot{q} = \frac{p}{m}, \tag{11}$$

$$\dot{p} = F - \frac{\xi p}{\tau}, \tag{12}$$

$$\dot{\xi} = \frac{(\langle p^2 \rangle / mkT) - 1}{\tau}. \tag{13}$$

- Disadvantages
  - Extended system not guaranteed to be ergodic
- Advantages
  - Easy to implement and use
  - Deterministic and time reversible

Nose-Hoover-Langevin Thermostat

- Controls temperature in a similar way that Nose dynamics
- Adds random noise to improve ergodicity
  - In contrast to Langevin dynamics, where noise is added directly to each physical degree of freedom, the new scheme relies on an indirect coupling to a single Brownian particle.

$$\frac{dq}{dt} = M^{-1}p \tag{14}$$

$$\frac{dp}{dt} = -\nabla V(q) - A(\xi)p \tag{15}$$

$$d\xi = \frac{1}{\mu}(p^t M^{-1} p - \frac{n}{\beta})dt - \frac{1}{2}\mu\beta\sigma^2\xi dt + \sigma dW \tag{16}$$

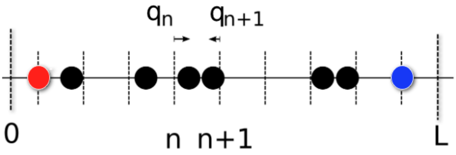
Fourier heat law

$$J = -\kappa \nabla T, \tag{17}$$

- Is there a microscopic foundation of Fourier's law?
- It is always valid?
- If so, under what conditions?

Description of the Model

- One-dimensional chain.



- Potential
  - Harmonic

$$\ddot{q}_n = q_{n+1} + q_{n-1} - 2q_n$$

  - Anharmonic FPU-β

$$\ddot{q}_n = q_{n+1} + q_{n-1} - 2q_n + \beta\left[(q_{n+1} - q_n)^3 - (q_n - q_{n-1})^3\right]$$

Chain system

$$\dot{q} = \frac{p}{m}$$

$$\dot{p} = q_{n+1} + q_{n-1} - 2q_n + \beta\left[(q_{n+1} - q_n)^3 - (q_n - q_{n-1})^3\right]$$

Nosee-Hoover thermostat

$$\dot{q} = \frac{p}{m}$$

$$\dot{p} = q_{n+1} + q_{n-1} - 2q_n + \beta\left[(q_{n+1} - q_n)^3 - (q_n - q_{n-1})^3\right] - \frac{\xi_n p_n}{\tau}$$

$$\dot{\xi} = \frac{(\langle p_n^2 \rangle / mkT) - 1}{\tau}$$

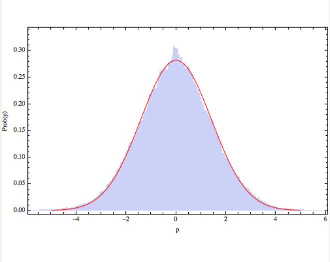
Discretization of the Stochastic differential equations

$$
\begin{aligned}
P &= p^n - \frac{\Delta t}{2}\nabla V(q^n), \\
Q &= q^n + \frac{\Delta t}{2} P, \\
P &= \exp(-\Delta t\, \xi^n/2) P, \\
\xi^{n+1} &= \xi^n + \frac{\Delta t}{\mu}\left(\sum \frac{P_i^2}{m_i} - \frac{n}{\beta}\right) + \sigma\sqrt{\Delta t} W - \frac{\Delta t\, \sigma^2}{4\mu}(\xi^n + \xi^{n+1}), \\
P &= \exp(-\Delta t\, \xi^{n+1}/2) P, \\
q^{n+1} &= Q + \frac{\Delta t}{2} P, \\
p^{n+1} &= P - \frac{\Delta t}{2}\nabla V(q^{n+1}).
\end{aligned}
$$

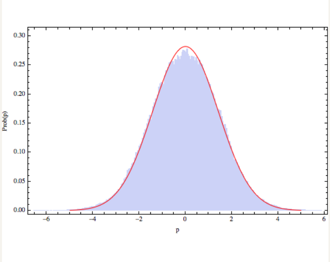
Table: Time averages for the thermostat temperatures

Deterministic	Stochastic
$\langle T \rangle_t$	$\langle T \rangle_t$
2.071738	2.060527

Deterministic thermostat



Stochastic thermostat

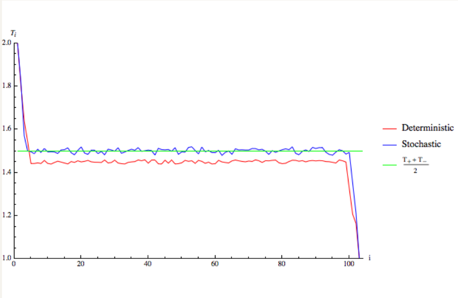


One-dimensional chain with harmonic interaction

- Theoretical result:

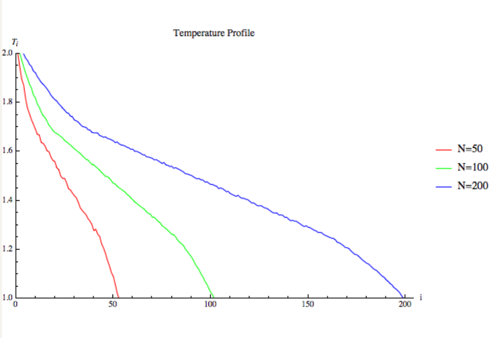
$$T = \frac{T_+ + T_-}{2} \tag{18}$$

Temperature profile

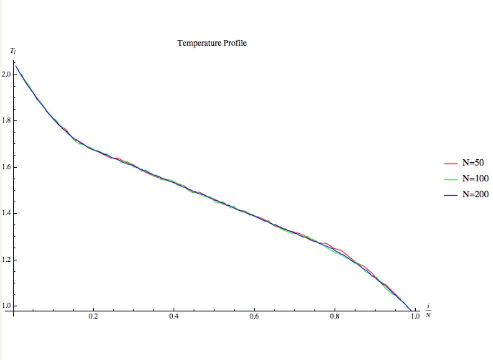


FPU-β chain

Temperature profile



Scaled temperature profile



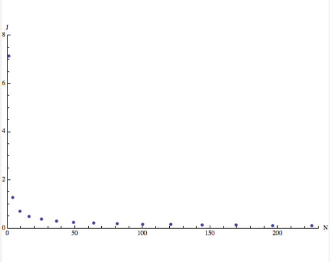
$$\frac{dT}{dx} \propto \frac{T^{+} - T_{-}}{N}$$

Heat flux

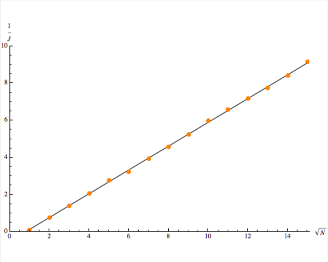
- The local heat flux $J(x,t)$ is defined by the continuity equation, details can be found in [6]:

$$J_i = \dot{x}_i \frac{\partial V}{\partial x_i}(x, x_{i+1}) \tag{19}$$

Heat flux



Scaling of the Heat flux



Furier law?

$$\kappa = \frac{J}{dT/dx} \tag{20}$$

- J scales to zero as $N^{-\alpha}$, with $\alpha \backsim 0.5$.
- The temperature gradient vanishes as N^{-1}.
- The conductivity diverges as $N^{1-\alpha}$

$$\Downarrow$$

FOURIER LAW IS NOT VALID FOR A FPU-β NONLINEAR CHAIN.

Relevance of computational modeling in complex system science

Existence of macro-equations for some dynamic systems

- We are typically interested in obtaining an explicit description or expression of the behavior of a whole system over time
- In the case of dynamical systems, this means solving their evolution rules, traditionally a set of differential equations (DEs)

Chemical kinetics

$$\frac{dA}{dt} = -\alpha k A^{\alpha} B^{\beta}$$

Wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla u$$

Existence of macro-equations and an analytical solution

- In some cases, the explicit formulation of an exact solution can be found by calculus, i.e., the symbolic manipulation of expressions

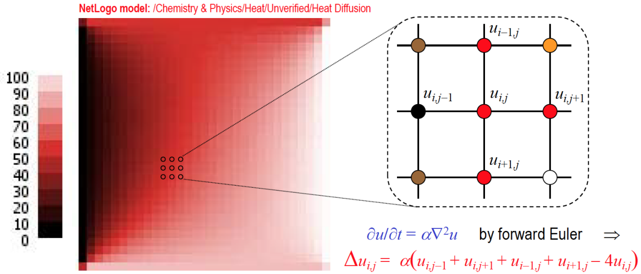
Heat equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad \text{with} \quad u(x,0) = \delta(x) \Longrightarrow u = \frac{1}{\sqrt{4\pi k t}} \exp\left(\frac{-x^2}{4kt}\right)$$

UNFORTUNATELY, ALTHOUGH VAST, THIS FAMILY IS IN FACT VERY SMALL COMPARED TO THE IMMENSE RANGE OF DYNAMICAL BEHAVIORS THAT NATURAL COMPLEX SYSTEMS CAN EXHIBIT!

Existence of macro-equations but no analytical solution

- When there is no symbolic resolution of an equation, numerical analysis involving algorithms (step-by-step recipes) can be used
- It involves the discretization of space into cells, and time into steps



Absence of macro-equations

- The physical world is a fundamentally nonlinear and out-of-equilibrium process
- Focusing on linear approximations and stable points is missing the big picture in most cases

No equations

Most real-world complex systems do not obey neat macroscopic laws

References

1. Guerin, S., Kunkle, D.: Emergence of Constraint in Self-Organizing Systems. NDPLS: Nonlinear Dynamics, Psychology, and Life Sciences 8 (2004) 131.
2. M. Dorigo, T. Stutzle, Ant Colony Optimazation, MIT Press 2004
3. Prigogine, I. Non-equilibrium statistical mechanics. New York: Wiley Interscience (1962).
4. Wm.G. Hoover, Time Reversibility, Computer Simulation, and Chaos, World Scientific, Singapore, 1999, 2001.
5. Chaos (2005) Focus issue 15, devoted to the FPU problem, AIP Journal.
6. Leimkuhler B, Noorizadeh E and Theil F 2009 J. Stat. Phys. 135 261–77
7. S. Lepri, R. Livi, and A. Politi, Physica D 119, 140 (1998).