Title: Boltzmann's Dog and Darwin's Finch: The statistical thermodynamics of self-replication and evolution

Date: Sep 17, 2014 02:00 PM

URL: http://pirsa.org/14090003

Abstract: Living things operate according to well-known physical laws, yet it is challenging to discern specific, non-trivial consequences of these constraints for how an organism that is a product of evolution must behave. Part of the difficulty here is that life lives very far from thermal equilibrium, where many of our traditional theoretical tools fail us. However, recent developments in nonequilibrium statistical mechanics may help light a way forward. The goal of this talk will be to explain some of these developments, and show how they begin to offer a new perspective on the physics of self-replication, natural selection, and evolution.

Boltzmann's Dog and Darwin's Finch

Jeremy England

Department of Physics
Massachusetts Institute of Technology

Wednesday, September 17, 2014
Perimeter Institute

The meaning of life

In biology we focus on

Behavior
Function
Survival
Reproduction
Heredity

We start by fiat: “That’s life.”

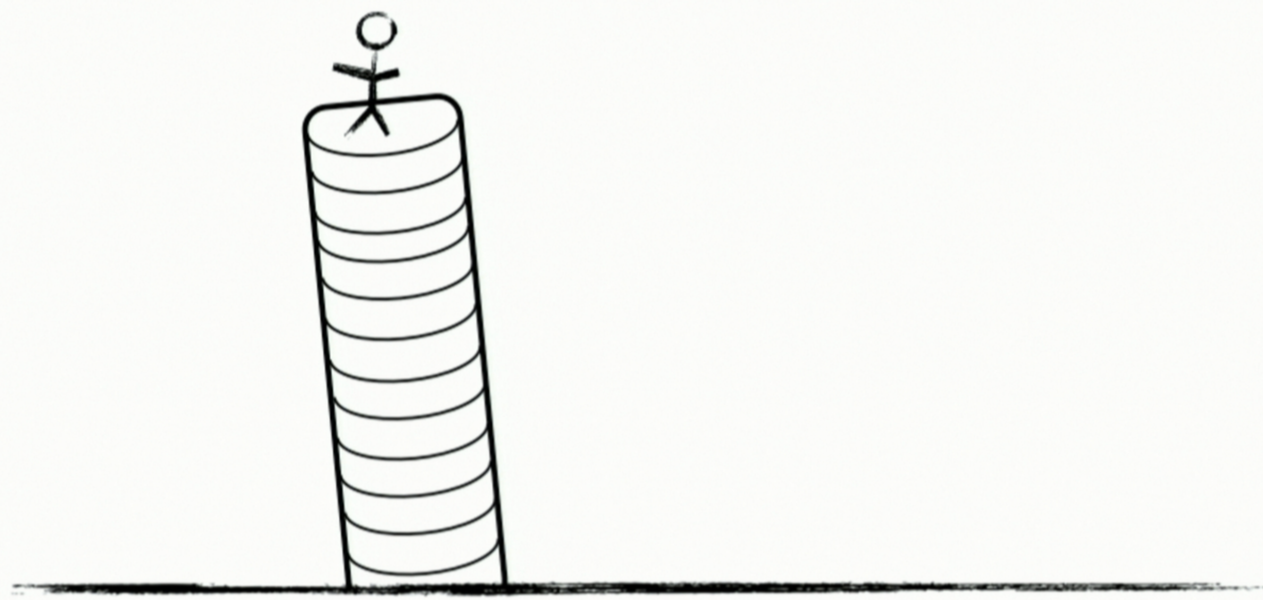
The meaning of physics

In physics we focus on

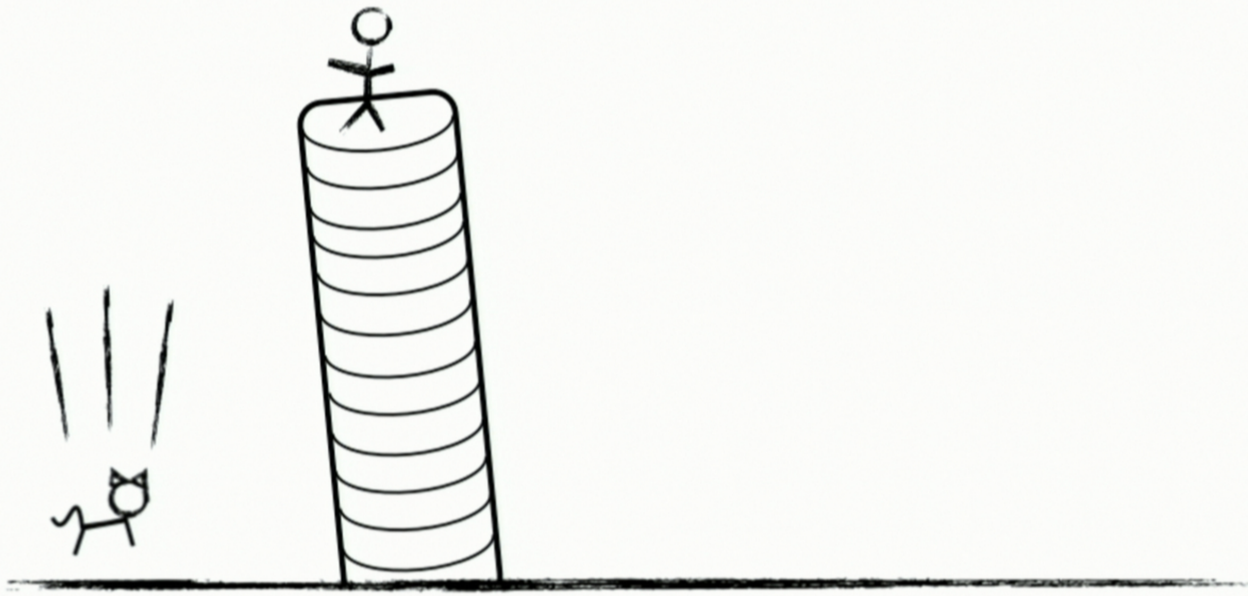
Distance (location)
Time
Number of particles
Energy
Temperature

A priori, life is absent from
the physical description

The art of translation

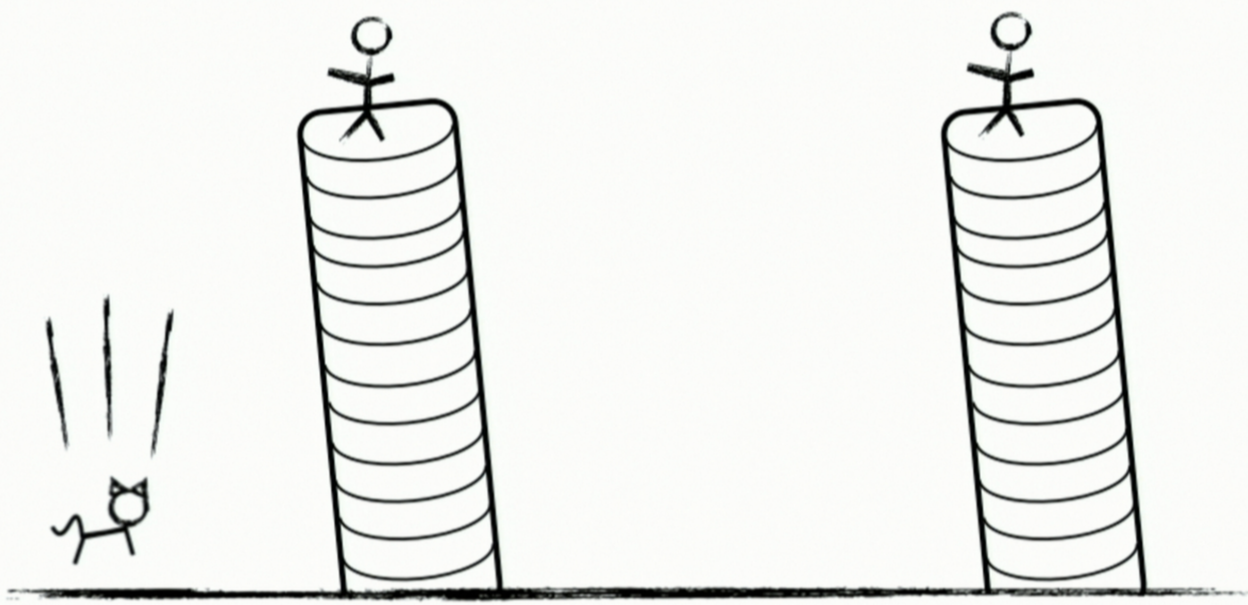


The art of translation



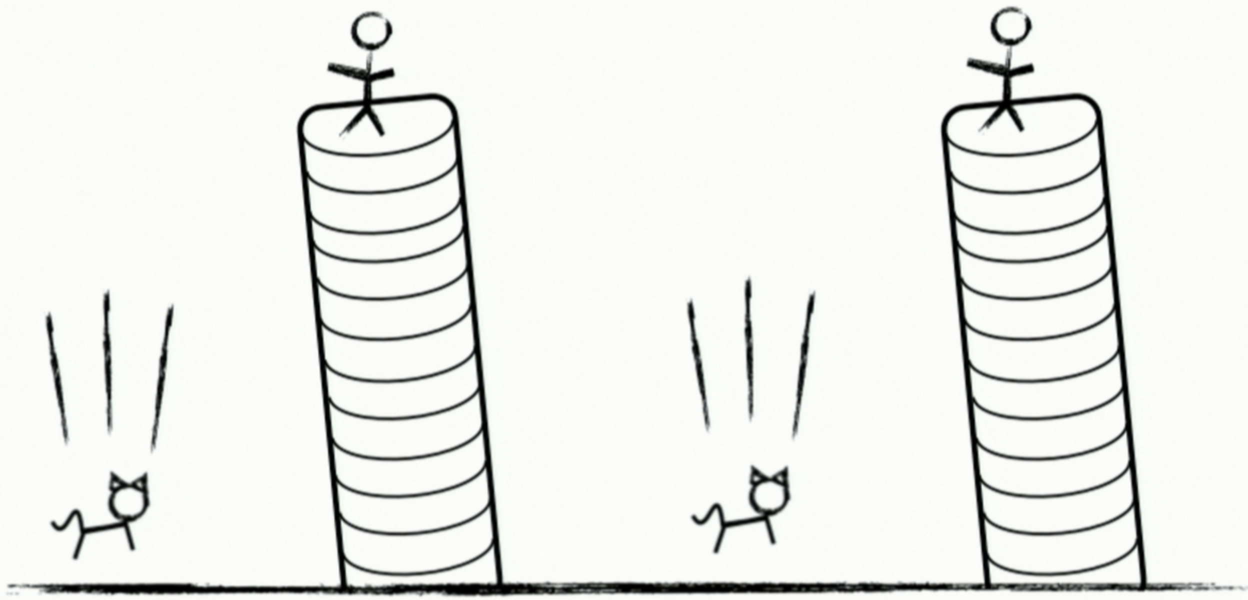
mv^2?

The art of translation



mv^2?

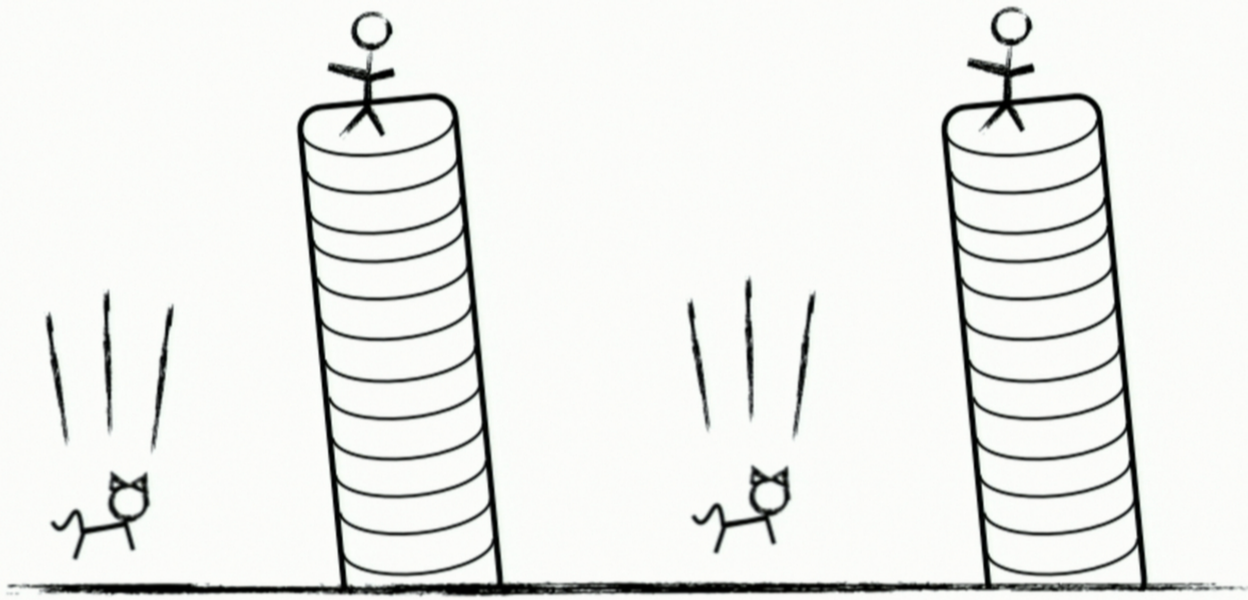
The art of translation



mv^2?

meow?

The art of translation



mv^2?
physics

Sometimes the link is clear

meow?
biology

What is special about life? ...(physically)

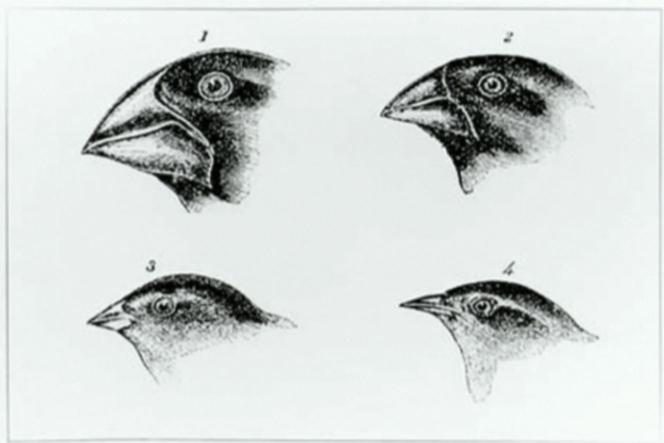
1 Self-replication

2 Sensing, computation, and anticipation

3 Effective absorption of work from environment

We tend to understand **3** and **2** in terms of **1**

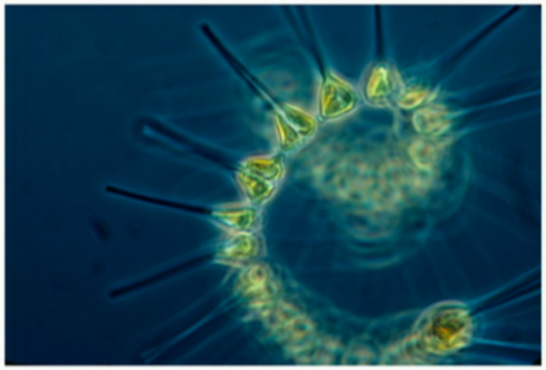
Fit Finch



"Fitness" is easiest to define when we are comparing replicators that are very similar

Darwin says the more rapid proliferator 'wins'

Fit Finch?



What really makes evolution
interesting is **adaptation**

Questions

Is there a general language for defining and understanding adaptation in physical terms?

Do we always need Darwinian selection to get adaptation?

Can we explain the emergence of life-like organization using fundamental physics?

Questions

Is there a general language for defining and understanding adaptation in physical terms? **Yes!**

Do we always need Darwinian selection to get adaptation? **No!**

Can we explain the emergence of life-like organization using fundamental physics? **Maybe?**

Hints

All living things are made of matter

All living things need to eat

All living things give off heat

All living things cannot grow backwards

Life and the arrow of time

Why is it so much more likely to see
a plant grow than ungrow?

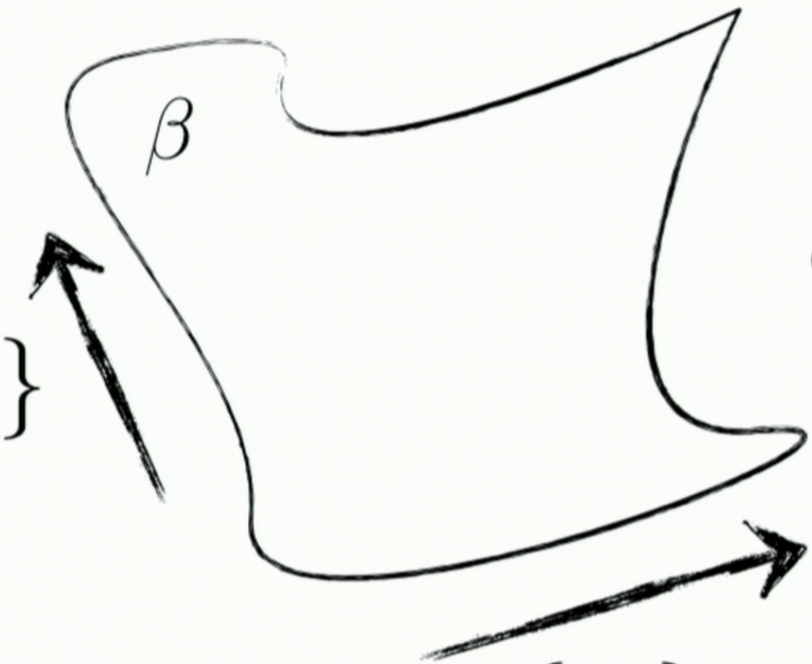
Life and the arrow of time

Why is it so much more likely to see
a plant grow than ungrow?

Hamiltonian dynamics

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q}$$



$\{q_i\}$

We explore a constant energy surface in phase space

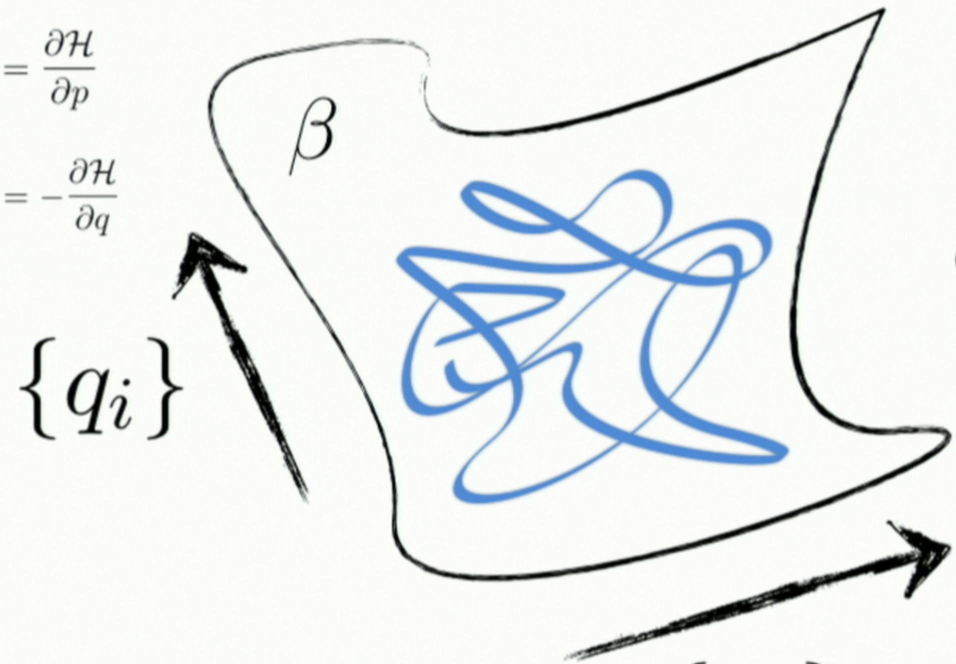
$\{p_i\}$

$$\beta = \frac{1}{T} = \frac{\partial \ln \Omega(E)}{\partial E}$$

Hamiltonian dynamics

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p}$$

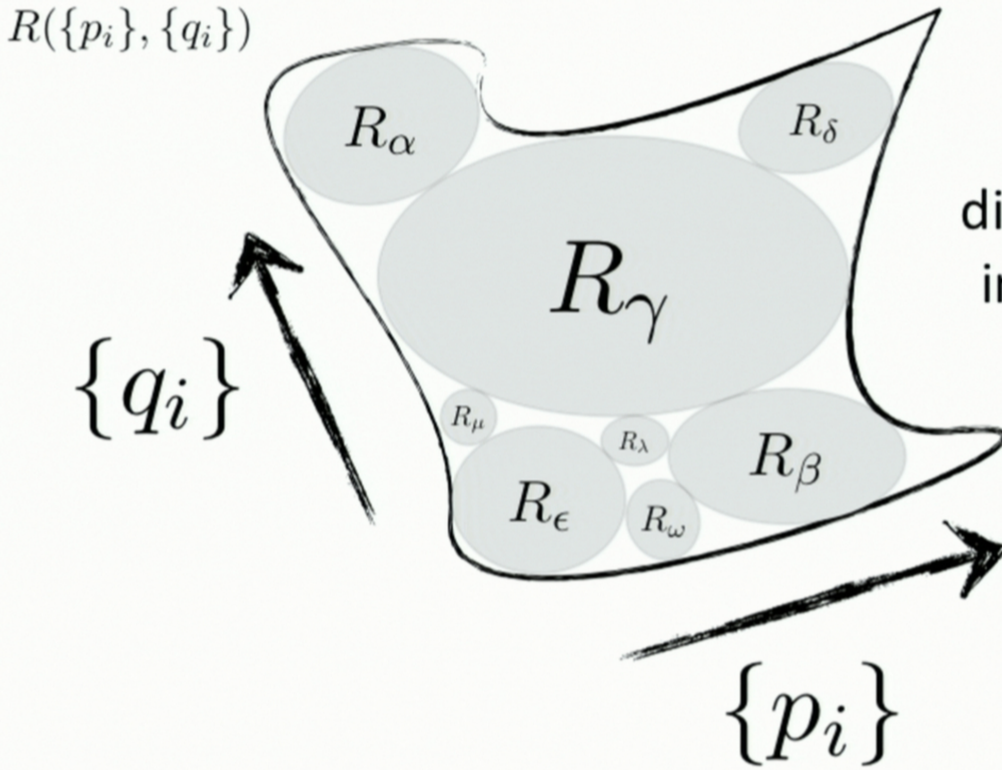
$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q}$$



We explore a constant energy surface in phase space

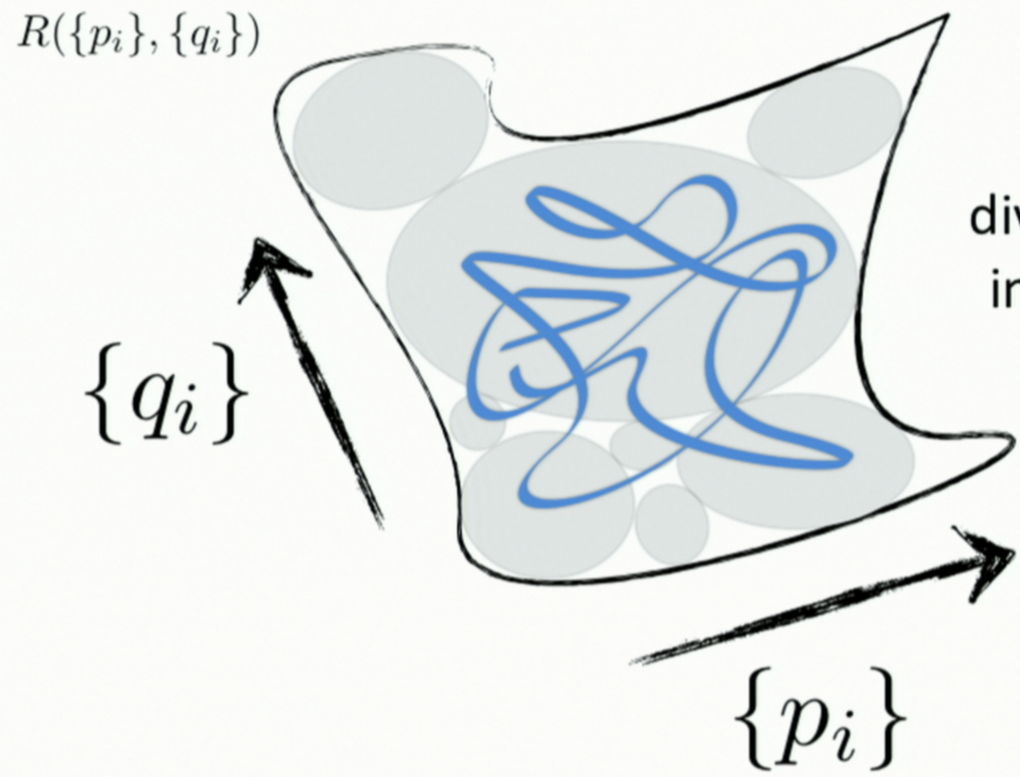
$$\beta = \frac{1}{T} = \frac{\partial \ln \Omega(E)}{\partial E}$$

Coarse-graining phase space



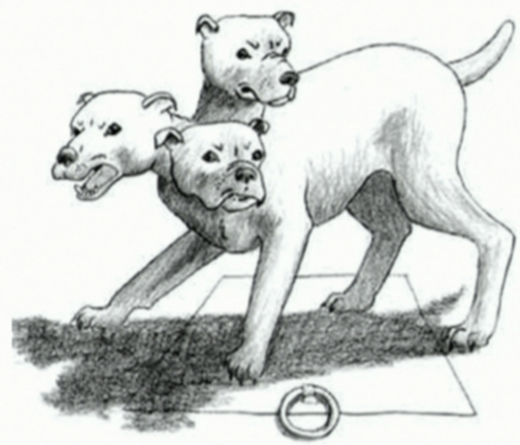
Our observable divides phase space into different sub-volumes

Coarse-graining phase space

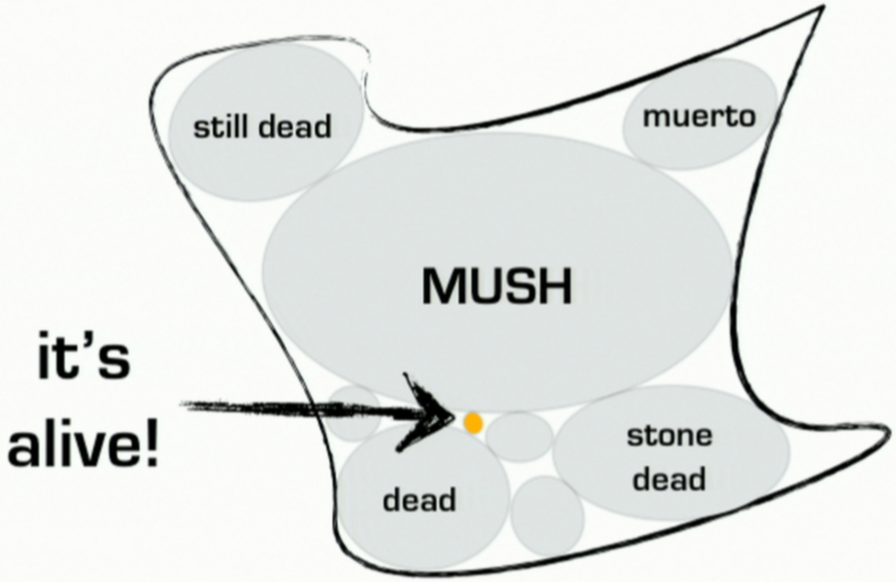


Our observable divides phase space into different sub-volumes

Boltzmann's Dog



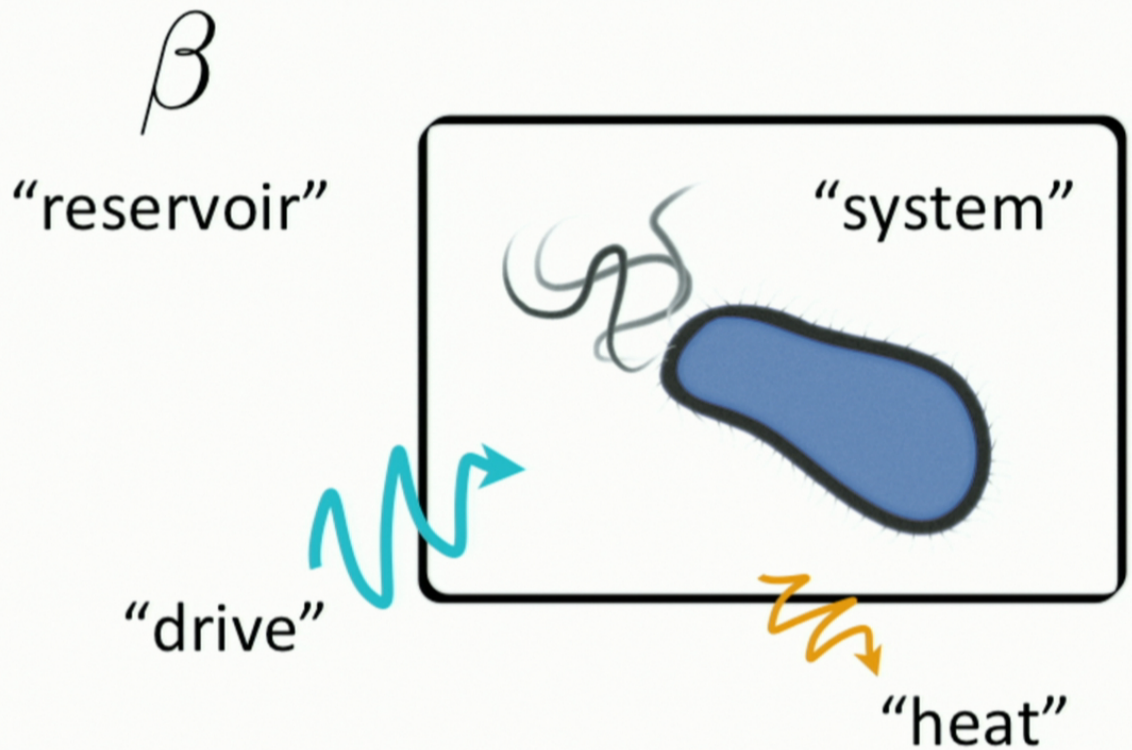
Boltzmann's Dog



The statistical equilibrium in a closed system is not going to be remotely alive

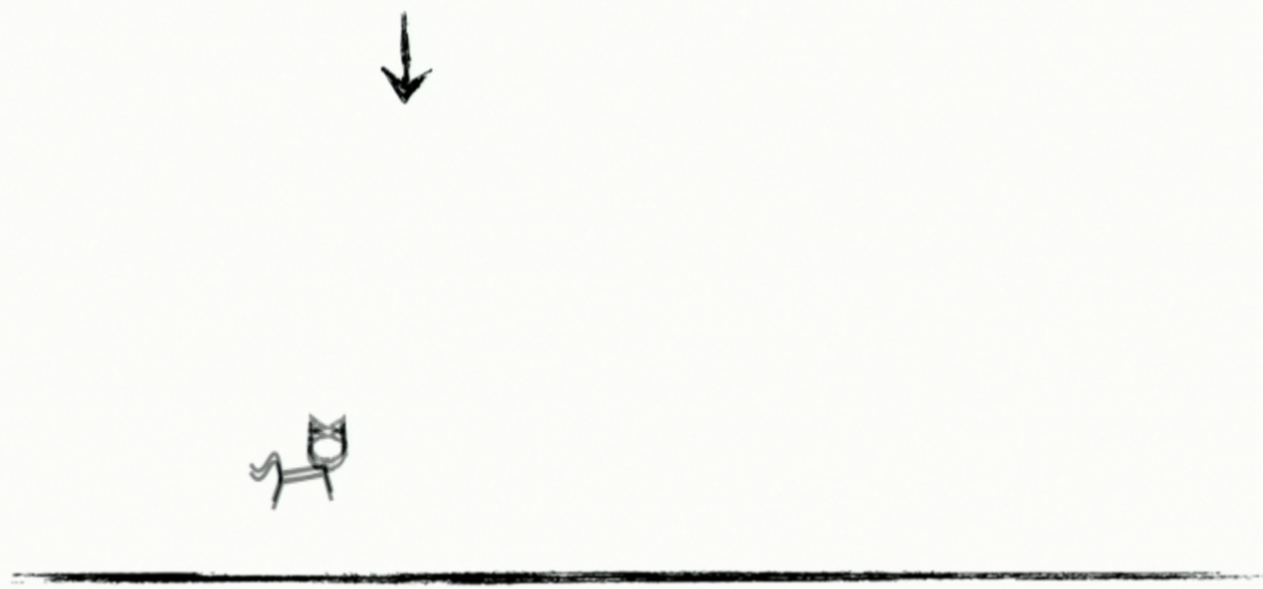
If living things are not at equilibrium then what can stat. mech. tell us?

Reservoir dogs

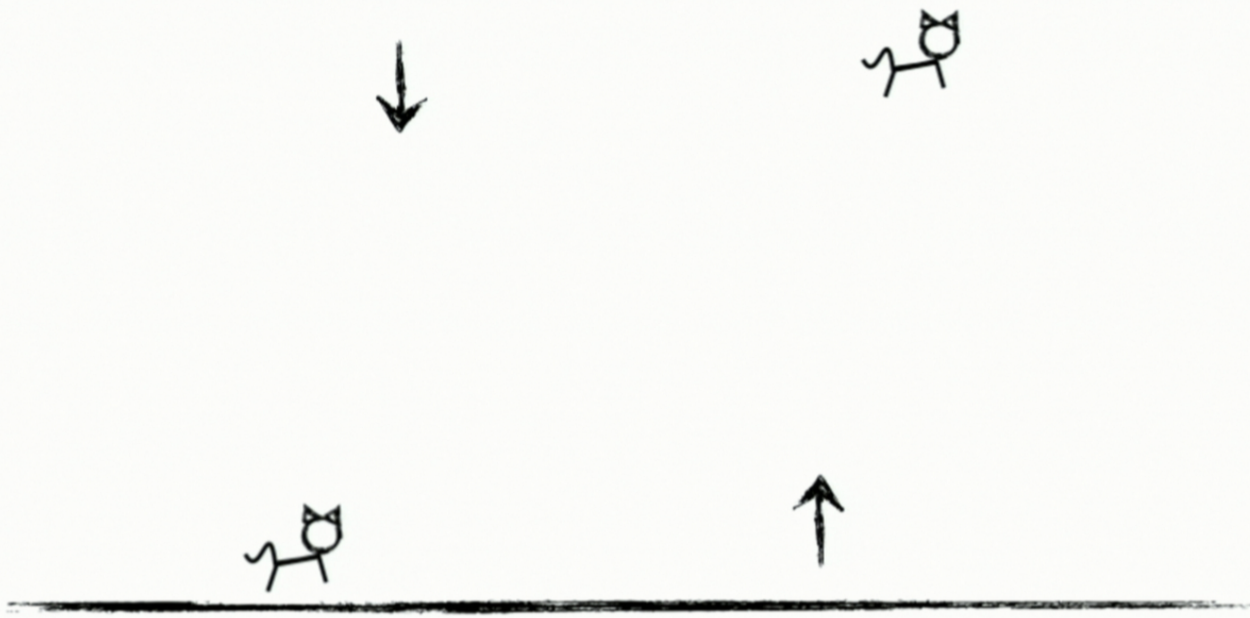


Newton's Laws and Symmetry

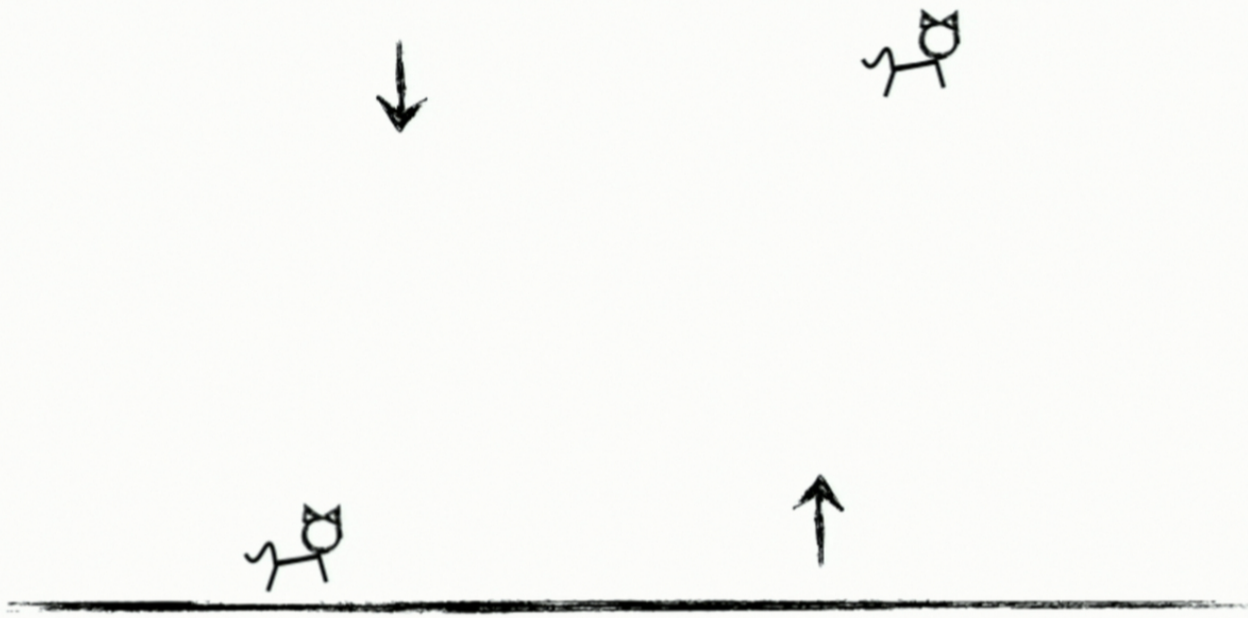
Newton's Laws and Symmetry



Newton's Laws and Symmetry



Newton's Laws and Symmetry



What goes up can come down

Detailed Balance

Time-reversal symmetry guarantees that detailed balance holds at thermal and chemical equilibrium

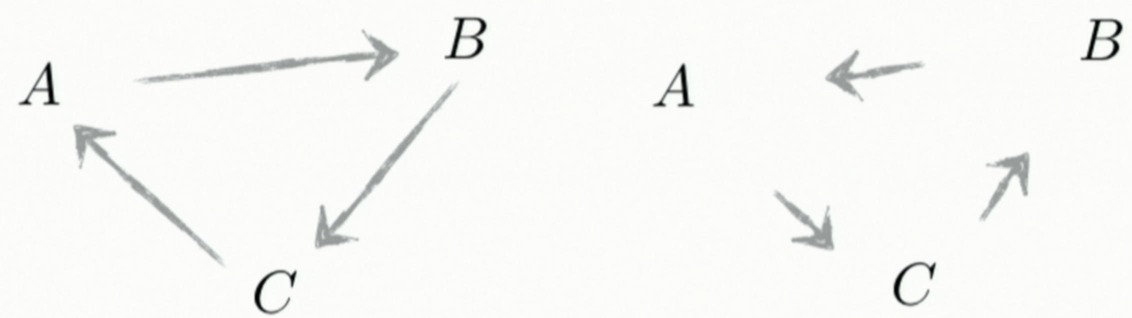
$$k_{A\to B}[A]_{eq} = k_{B\to A}[B]_{eq} \qquad \frac{k_{A\to B}}{k_{B\to A}} = \frac{[B]_{eq}}{[A]_{eq}} \equiv K_{eq}^{BA}$$

$$k_{C\to B}[C]_{eq} = k_{B\to C}[B]_{eq} \qquad \frac{k_{C\to B}}{k_{B\to C}} = \frac{[B]_{eq}}{[C]_{eq}} \equiv K_{eq}^{BC}$$

$$k_{C\to A}[C]_{eq} = k_{A\to C}[A]_{eq} \qquad \frac{k_{C\to A}}{k_{A\to C}} = \frac{[A]_{eq}}{[C]_{eq}} \equiv K_{eq}^{AC}$$

Detailed Balance-Breaking

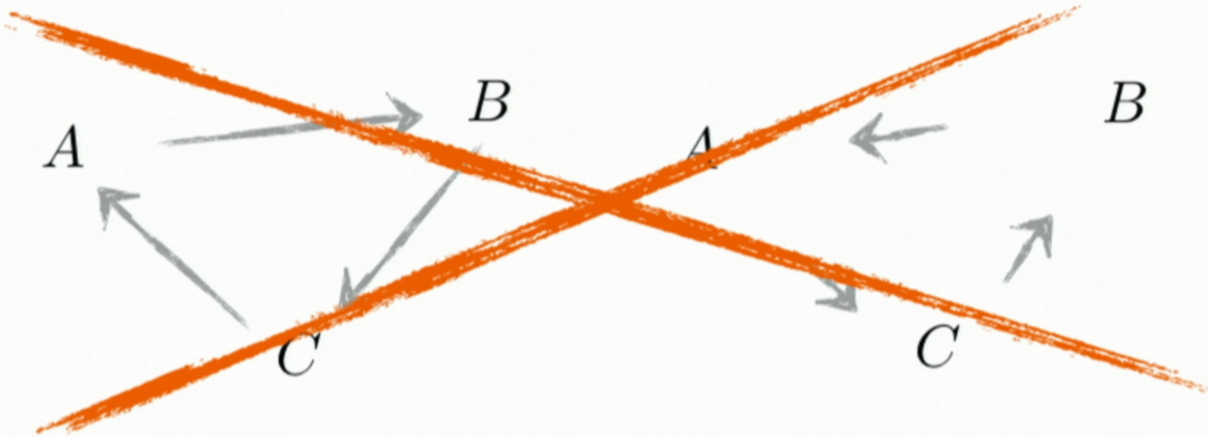
Net reaction cycles are forbidden at equilibrium!



$$k_{A\to B}[A]_{eq} \neq k_{B\to A}[B]_{eq}$$

Detailed Balance-Breaking

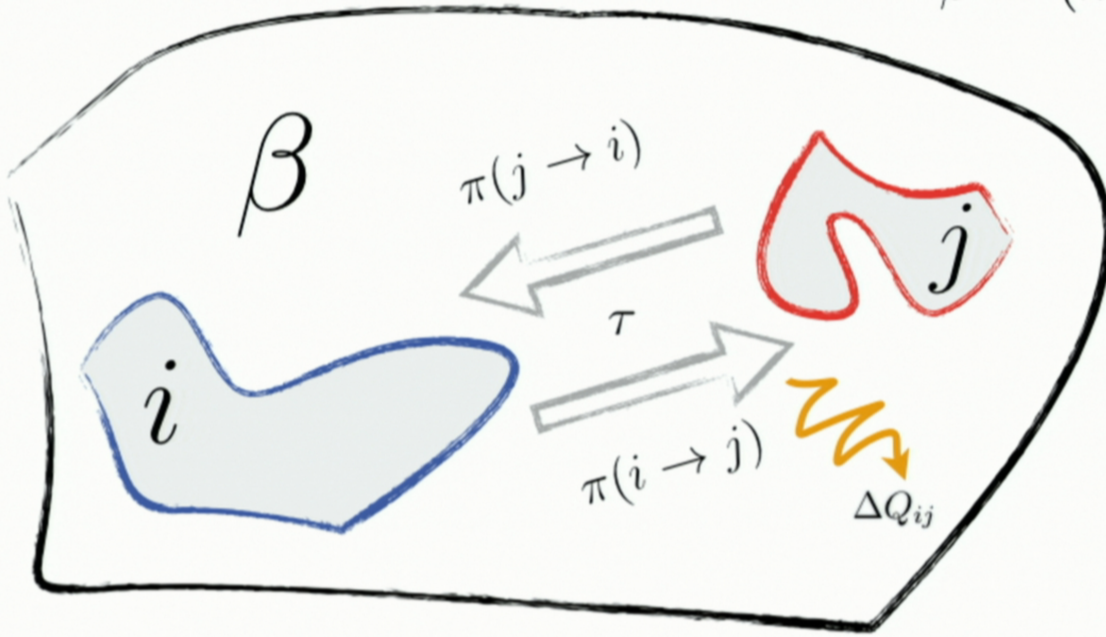
Net reaction cycles are forbidden at equilibrium!



$$k_{A\to B}[A]_{eq} \neq k_{B\to A}[B]_{eq}$$

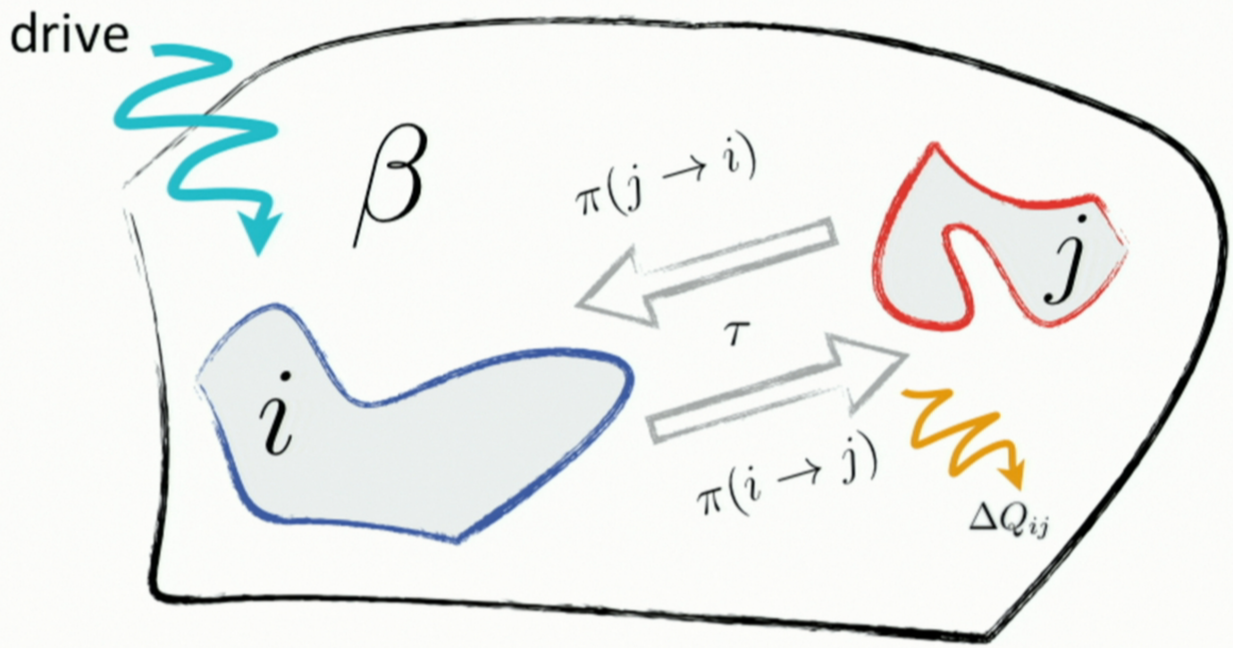
Back and Forth

$$\beta \equiv (k_B T)^{-1}$$



$$\frac{\pi(j \to i)}{\pi(i \to j)} = \exp[-\beta(E_i - E_j)] = \exp[-\beta \Delta Q_{ij}]$$

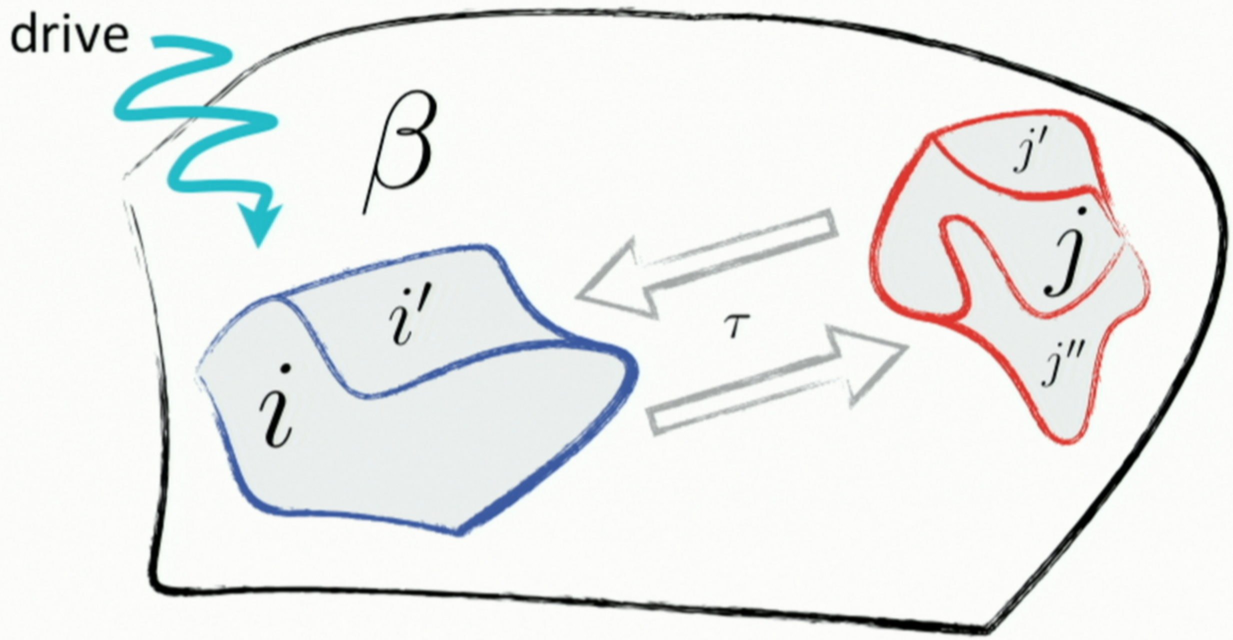
Irreversibility and Entropy



$$\frac{\pi(j \to i)}{\pi(i \to j)} = \langle \exp[-\beta \Delta Q_{ij}] \rangle_{i \to j}$$

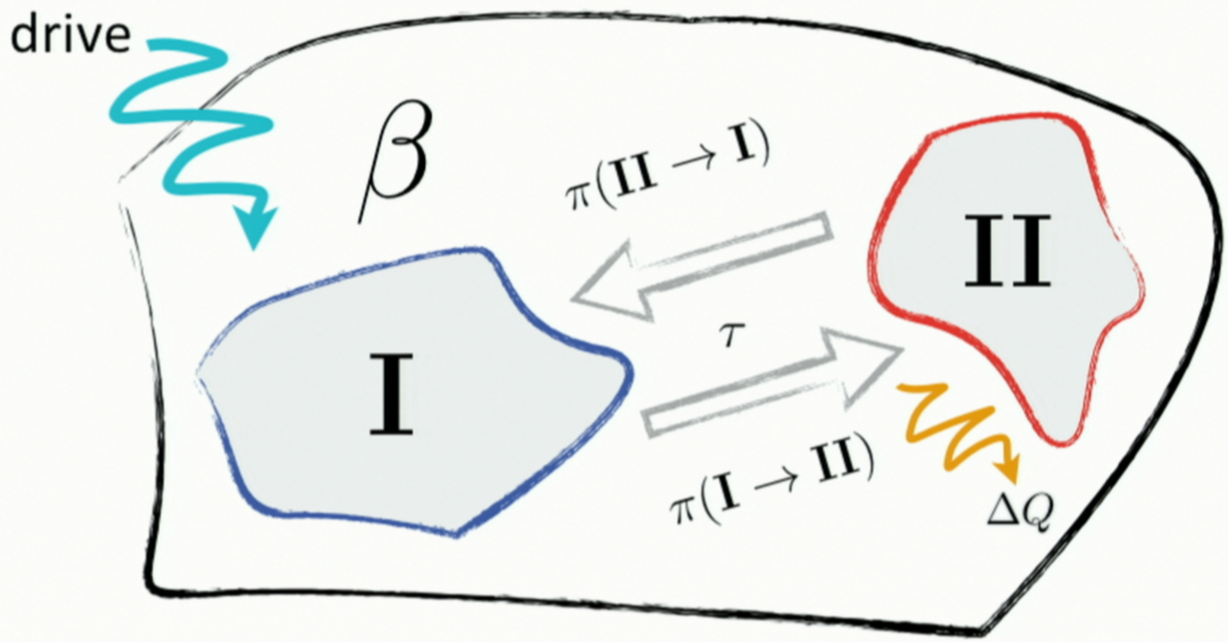
Crooks, 1999

Macrostate Construction



$$\mathbf{I} : i, i''' \qquad \mathbf{II} : j, j', j''$$

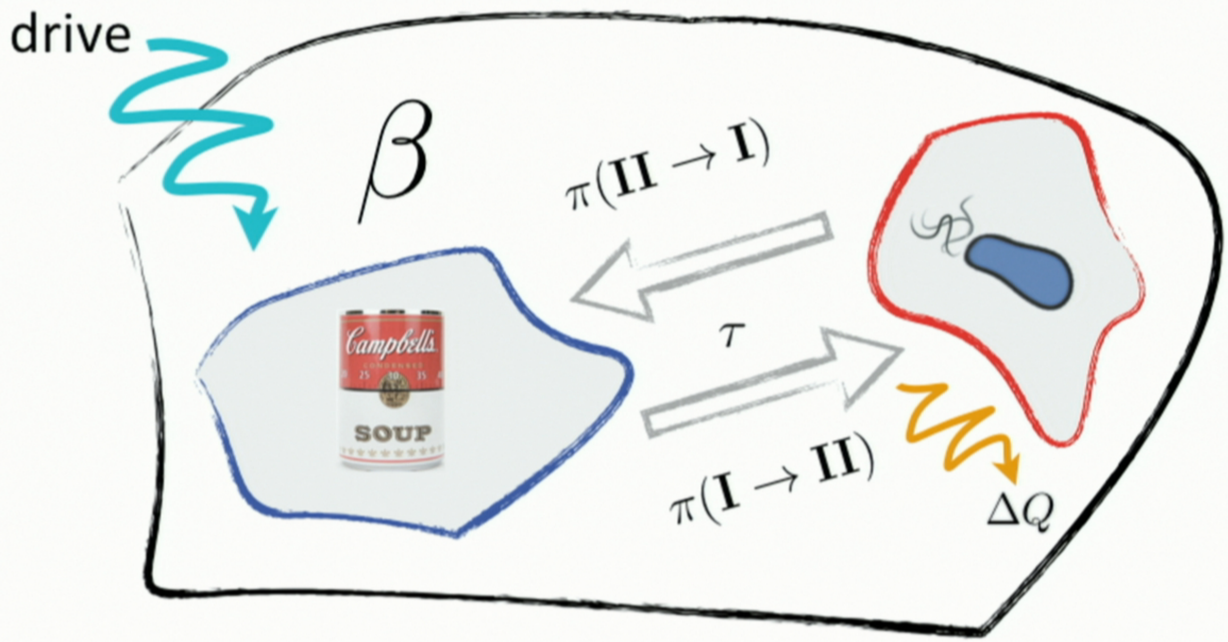
Macrostate Construction



$\mathbf{I} : i, i'''$ $\quad$ $\mathbf{II} : j, j', j''$

$p(i|\mathbf{I})$ $\quad$ $p(j|\mathbf{II})$

Macrostate Construction

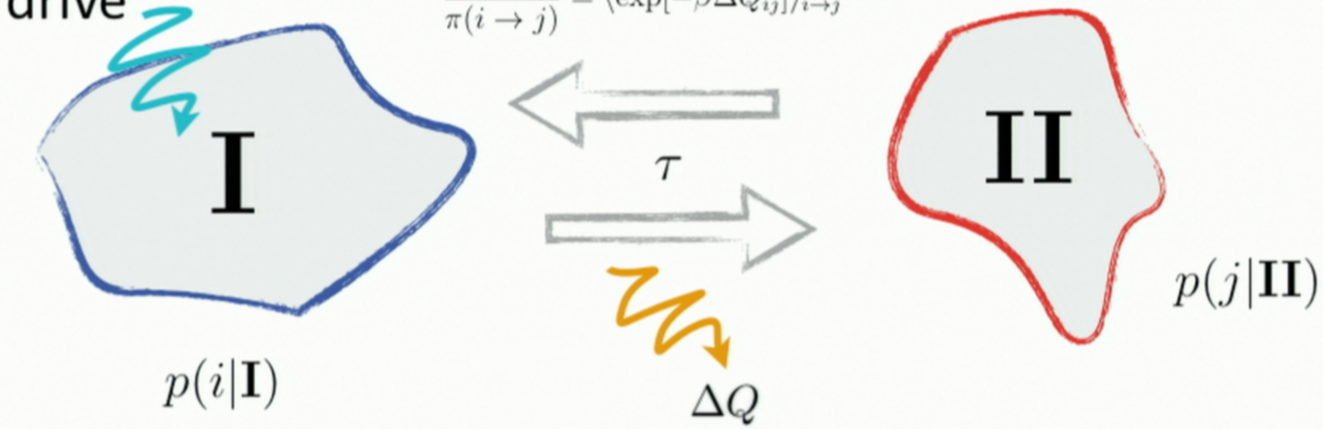


"Die Grenzen meiner Sprache
bedeuten die Grenzen meiner Welt."

Wittgenstein, 1922

Irreversibility, Entropy, and Macrostates

$$\frac{\pi(j \to i)}{\pi(i \to j)} = \langle \exp[-\beta \Delta Q_{ij}] \rangle_{i \to j}$$



England, 2013

$$\frac{\pi(\mathbf{II} \to \mathbf{I})}{\pi(\mathbf{I} \to \mathbf{II})} = \left\langle e^{\ln\left[\frac{p(j|\mathbf{II})}{p(i|\mathbf{I})}\right]} \langle e^{-\beta \Delta Q_{i \to j}} \rangle_{i \to j} \right\rangle_{\mathbf{I} \to \mathbf{II}}$$

Jensen and the Second Law

$$e^x \geq x + 1$$

$$\langle e^x \rangle \geq \langle x \rangle + 1$$

$$\frac{\pi(\mathbf{II} \to \mathbf{I})}{\pi(\mathbf{I} \to \mathbf{II})} = \left\langle e^{-\Delta S_{total}} \right\rangle_{\mathbf{I} \to \mathbf{II}}$$

$$\Delta S_{total} \geq \ln \left[\frac{\pi(\mathbf{I} \to \mathbf{II})}{\pi(\mathbf{II} \to \mathbf{I})} \right]$$

Jensen and the Second Law

$$\Delta S_{tot} = \beta\langle \Delta Q \rangle + \Delta S_{int} \geq \ln\left[\frac{\pi(\mathbf{I} \to \mathbf{II})}{\pi(\mathbf{II} \to \mathbf{I})}\right] \geq 0$$

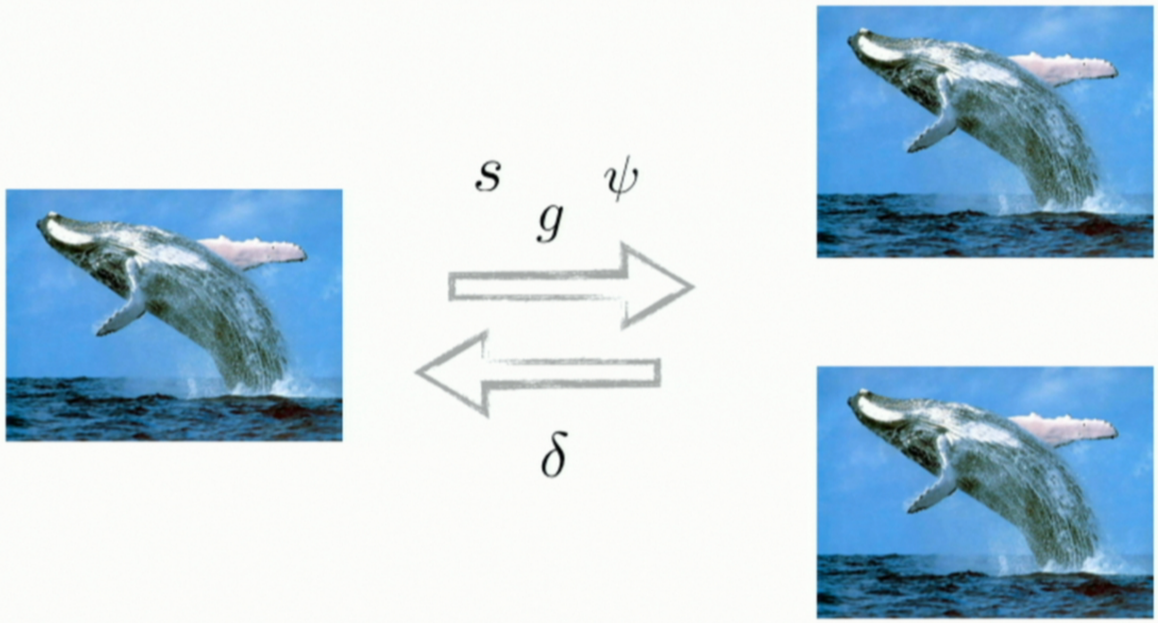
Entropy production tracks with irreversibility at a macroscopic level, even when driven far from equlibrium!

This is true for arbitrary coarse-grainings, including

bit erasure/computing (Laundauer)
Markov processes (Blythe)
chemical reactions (Prigogine & DeDonder) . . .

. . . and for **self-replication**

Growth and dissipation



Growth is accompanied by internal
entropy change and dissipation

Growth and dissipation

g exponential growth rate

δ spontaneous reversal rate

s system entropy change

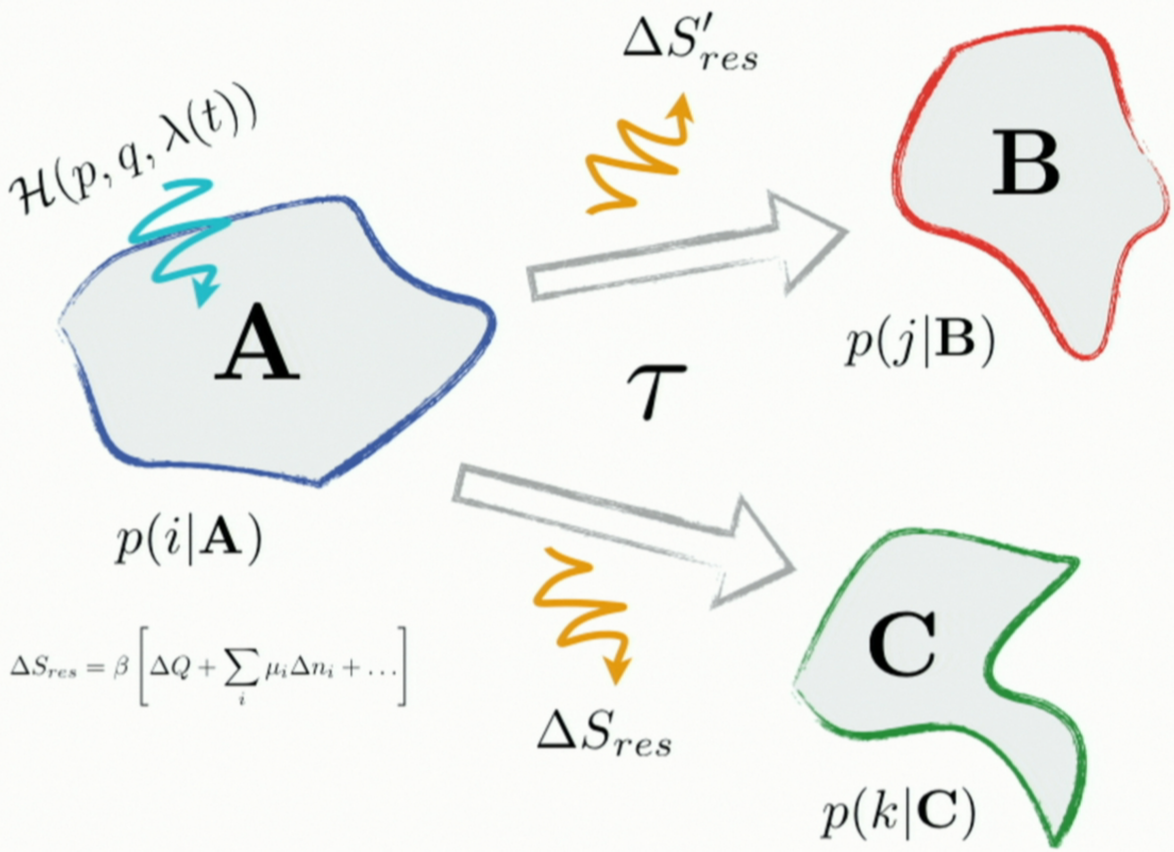
ψ dissipation in reservoir

Doubling time will be roughly proportional to $1/(g-\delta)$

$\psi \geq \ln[g/\delta] - s$ is generally going to be positive

So, winning Darwin's game happens to be about dissipating more than your competitor

Driven Stochastic Evolution



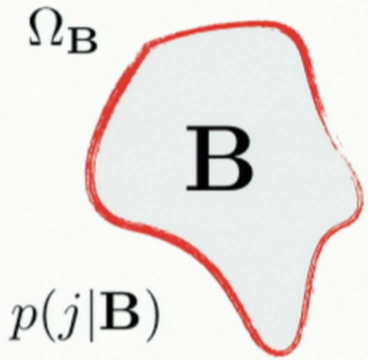
$$\Delta S_{res} = \beta \left[\Delta Q + \sum_i \mu_i \Delta n_i + \ldots \right]$$

Driven Stochastic Evolution

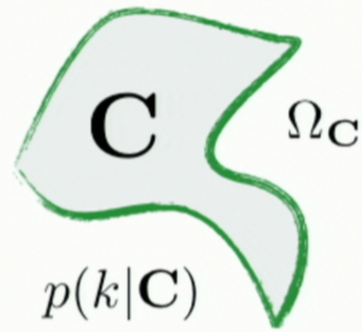
$$\ln\left[\frac{\pi(\mathbf{A}\to\mathbf{B})}{\pi(\mathbf{A}\to\mathbf{C})}\right] \simeq \Delta\ln\Omega_{\mathbf{BC}} + \ln\left[\frac{\pi(\mathbf{B}\to\mathbf{A})}{\pi(\mathbf{C}\to\mathbf{A})}\right] - \ln\left[\frac{\langle\exp[-\Delta S_{res}]\rangle_{\mathbf{A}\to\mathbf{B}}}{\langle\exp[-\Delta S_{res}]\rangle_{\mathbf{A}\to\mathbf{C}}}\right]$$

order **durability** **fluctuation and dissipation**

Coming to terms



Compare phase space volumes of the two macrostates



$$\Delta \ln \Omega_{\mathbf{BC}} \simeq -\sum_k p(j|\mathbf{B}) \ln p(j|\mathbf{B}) + \sum_k p(k|\mathbf{C}) \ln p(k|\mathbf{C})$$

Systems coupled to reservoirs tend to get more disordered because of fluctuations

Coming to terms

$$-\ln\langle\exp[-\Delta S]\rangle = \langle\Delta S\rangle - \frac{\sigma^2_{\Delta S}}{2} + \ldots$$

$$-\ln\langle\exp[-\Delta S]\rangle \equiv \Psi - \Phi$$

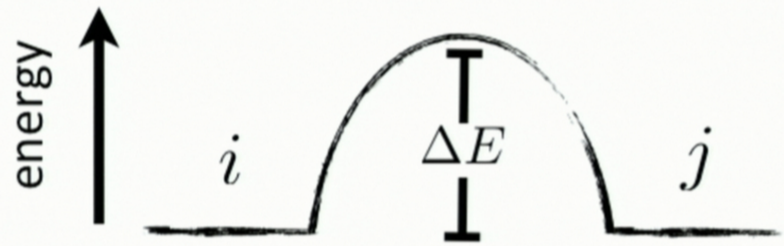
Cumulant generating function breaks into two pieces:
the **mean dissipation**, and the **fluctuations** about the mean

(**Warning:** Fluctuations can dominate!)

To make this quantity very positive,
you need **reliably** high dissipation

Intuition from Arrhenius

Where does the relationship between dissipation in the reservoir and likelihood come from?

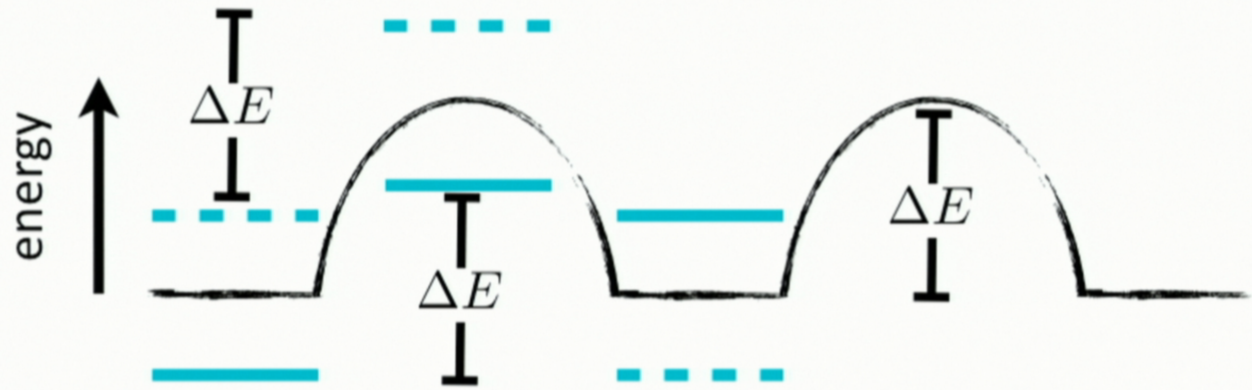


Transition rates are controlled by activation barrier heights

$$k_{i\to j} = k_0 e^{-\Delta E/k_B T}$$

Intuition from Arrhenius

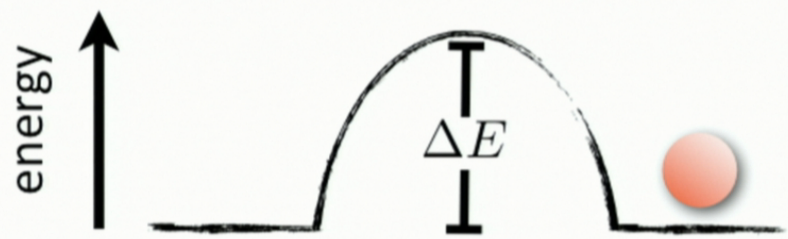
The effect of a time-varying external drive is to oscillate the energies of different microstates



Concerted drift is produced by events that tend to absorb work from the external drive

Intuition from Arrhenius

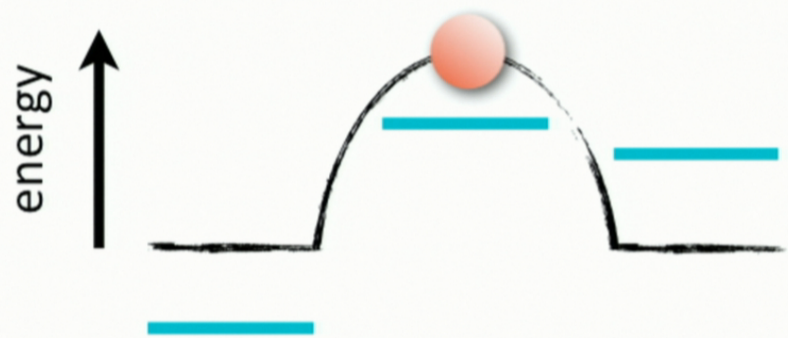
We start out at the beginning of a drive cycle in the state on the right



We assume the barrier is high enough that we are unlikely to cross from thermal fluctuations alone

Intuition from Arrhenius

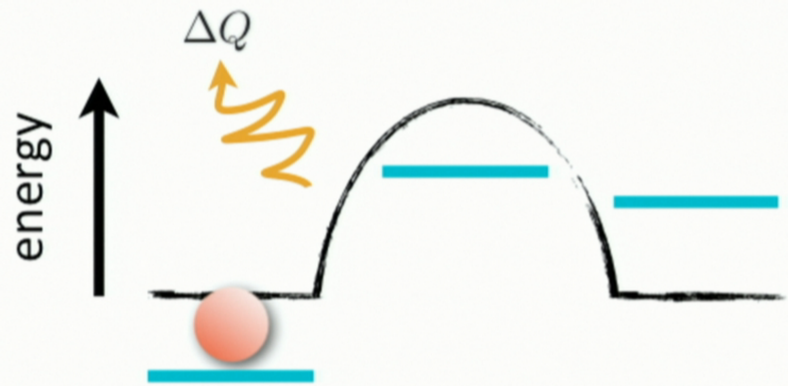
Then the drive lifts us up in energy by doing work



The likelihood of hopping over to the transition state from thermal fluctuation becomes much higher

Intuition from Arrhenius

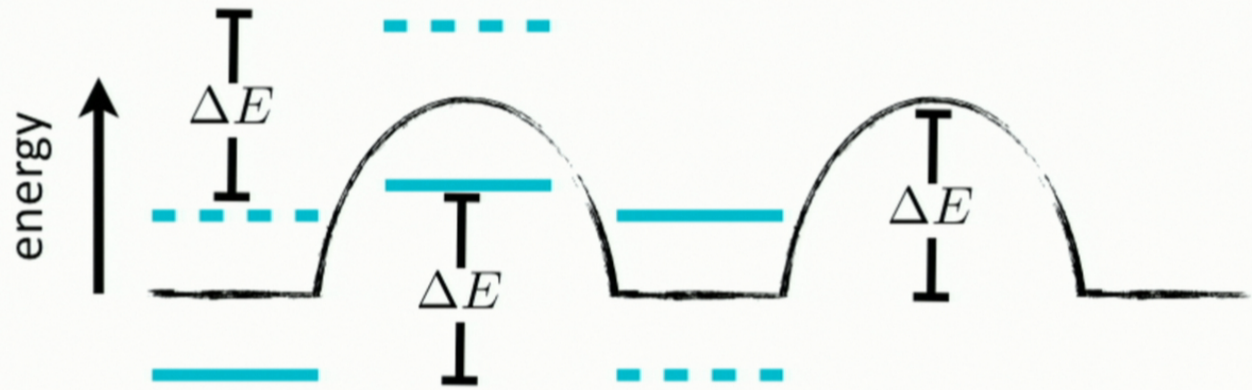
Then the drive lifts us up in energy by doing work



The likelihood of hopping over to the transition state from thermal fluctuation becomes much higher

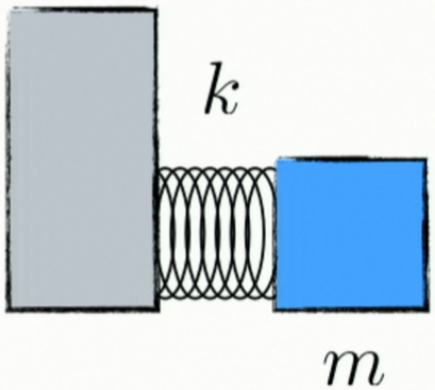
Intuition from Arrhenius

Comparing states of fixed return probability is essential



On such a surface of states, dissipation and drift are coupled

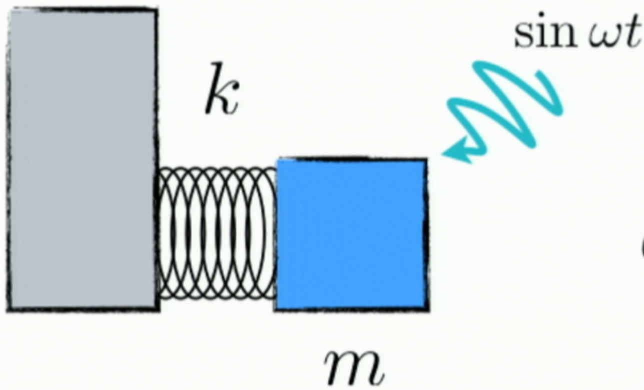
Oscillation and Resonance



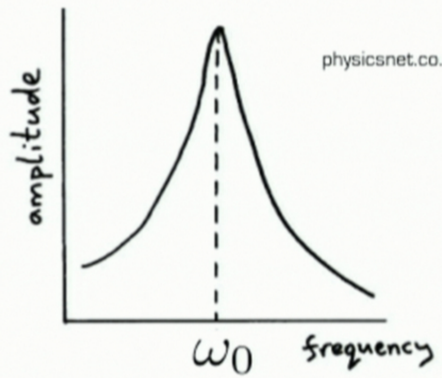
$$\omega_0 = \sqrt{k/m}$$

The same mechanical system moves more when it is driven at the right frequency

Oscillation and Resonance

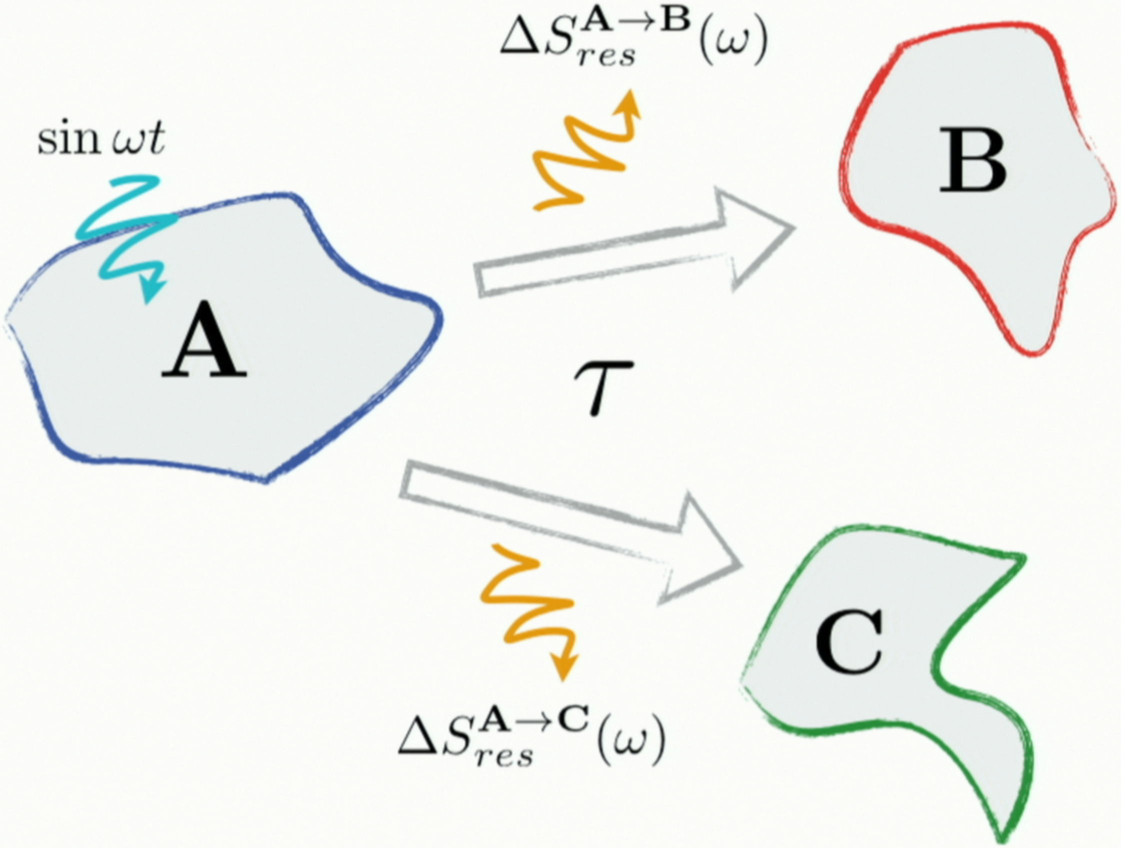


$$\omega_0 = \sqrt{k/m}$$



The same mechanical system moves more when it is driven at the right frequency

Driven Stochastic Evolution



Lessons from Skiing

What happens when you wander through a mountain range covered by a random assortment of ski lifts?

Where do you eventually end up after a long time?

Lessons from Skiing

For a given external drive, some arrangements of matter will resonate more and absorb more energy

This is like a region where there are more ski lifts

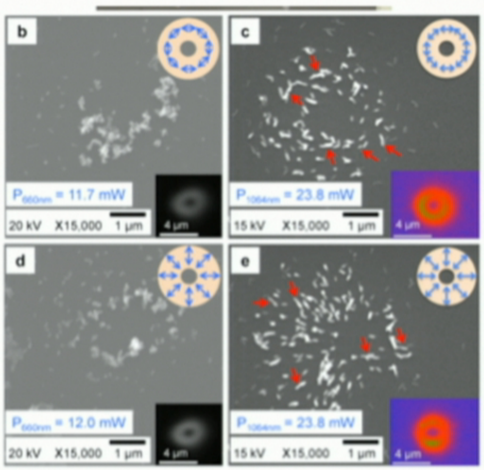
Sometimes we ride up one side of the mountain and ski down the other

The more this happens, the more we get trapped in shapes that form by being specially adapted to the drive

Not your typical macrostate

Living things are good at getting applied fields to do work on them so they can dissipate the energy

Resonant Adaptation

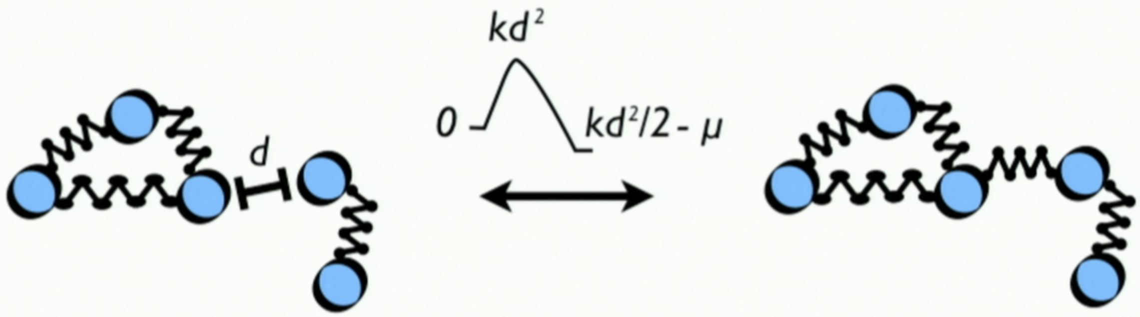


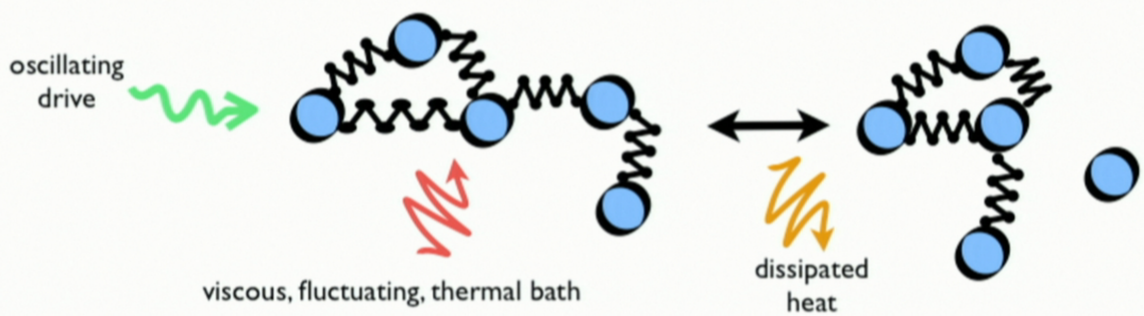
Ito et al., Scientific Reports, 2013

Silver nanorods self-assemble into structures that match surface plasmon resonance to wavelength of driving light field

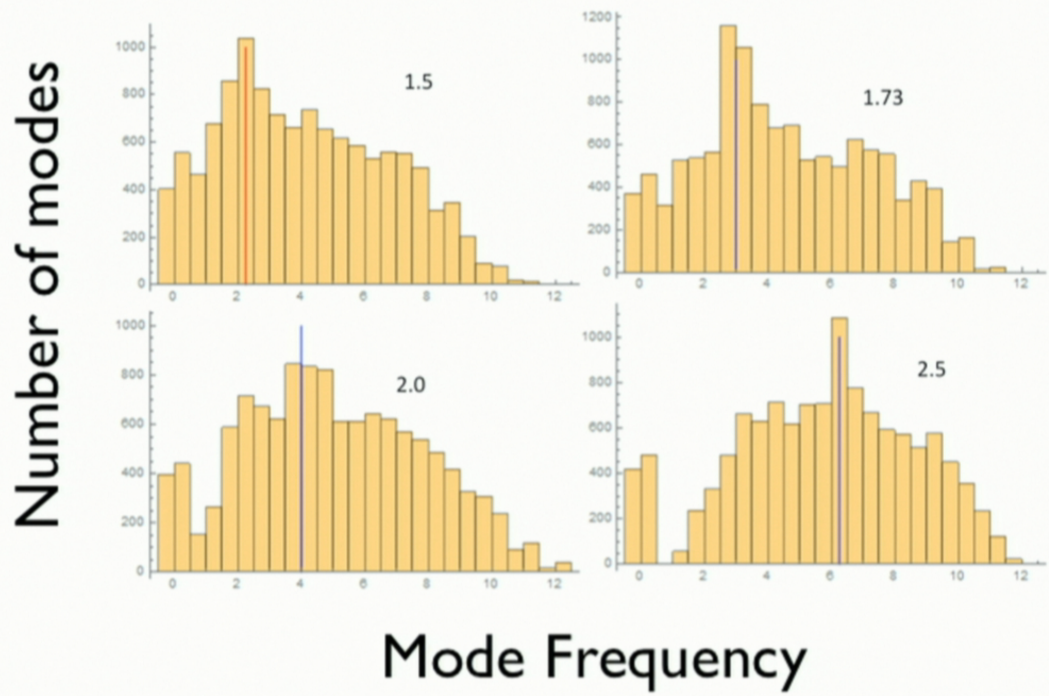
No need to talk about anything in the system making a copy of itself . . .

Spontaneous Rewiring





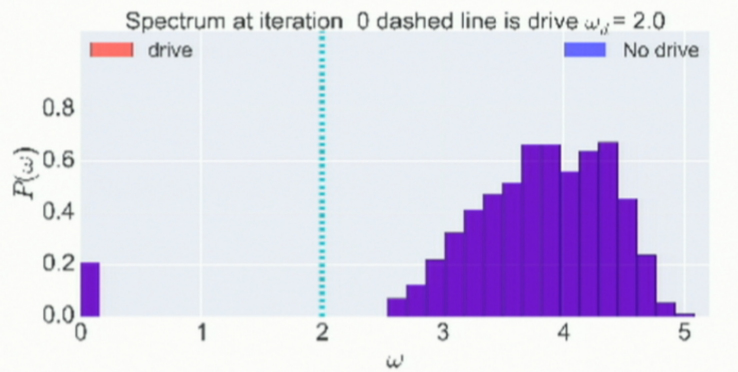
Adaptation without Selection

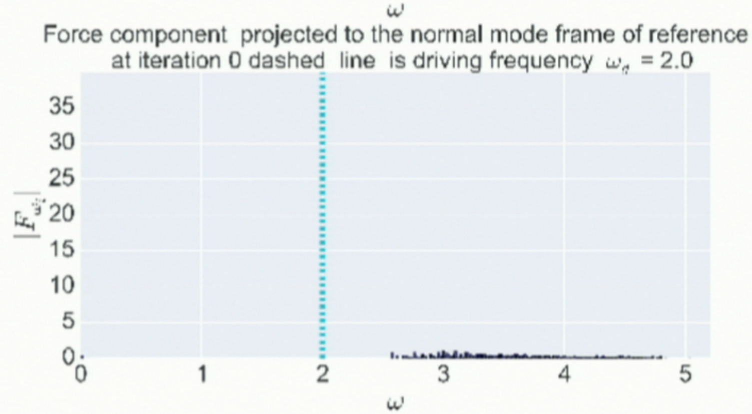


Adaptation without Selection

As time passes network resonates more with drive

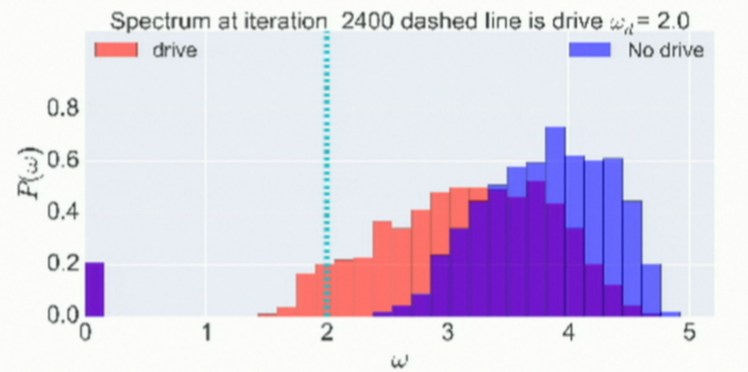
Springs rearrange to absorb more work from single driven particle



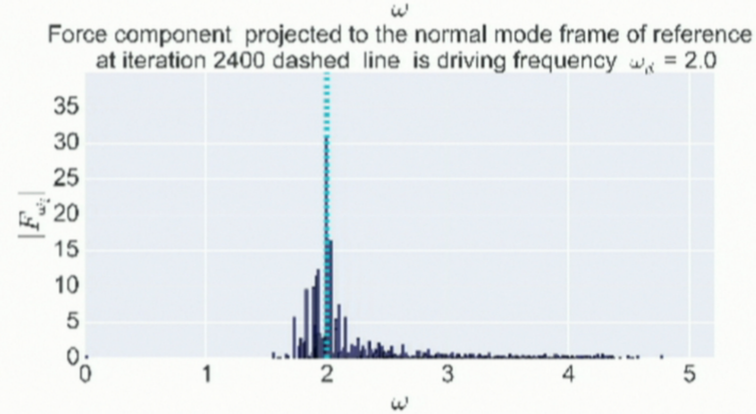


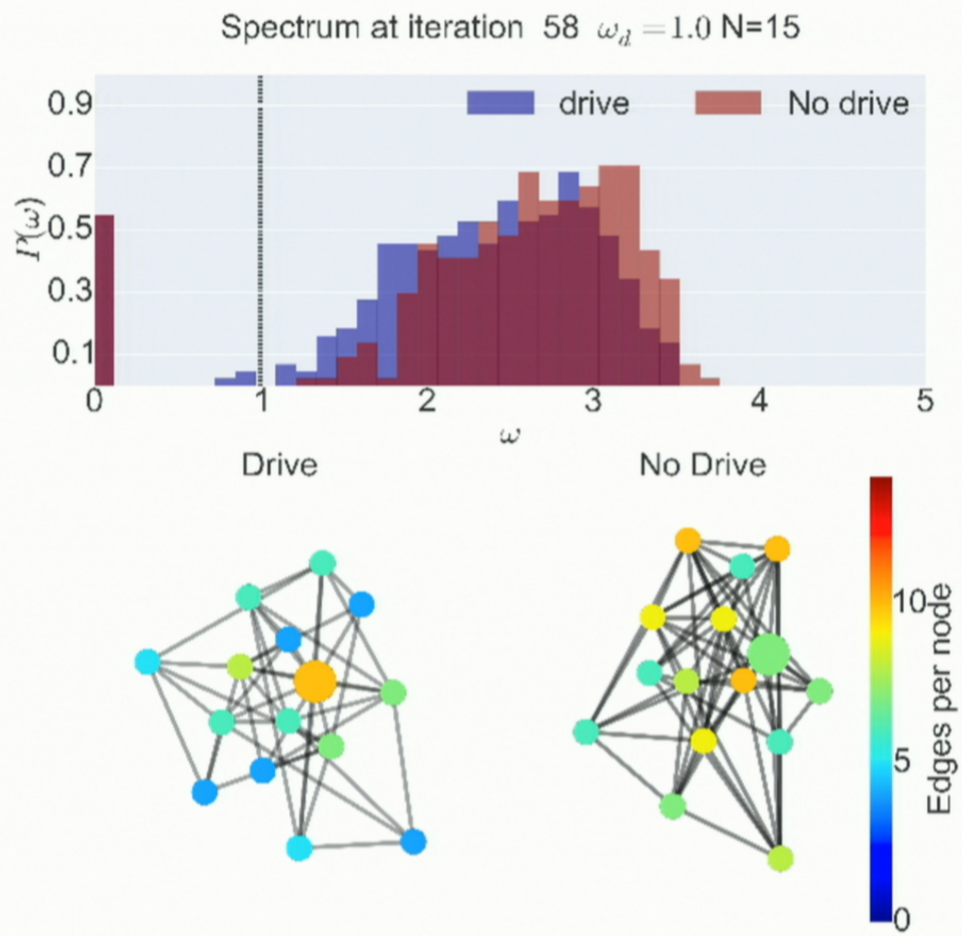
Adaptation without Selection

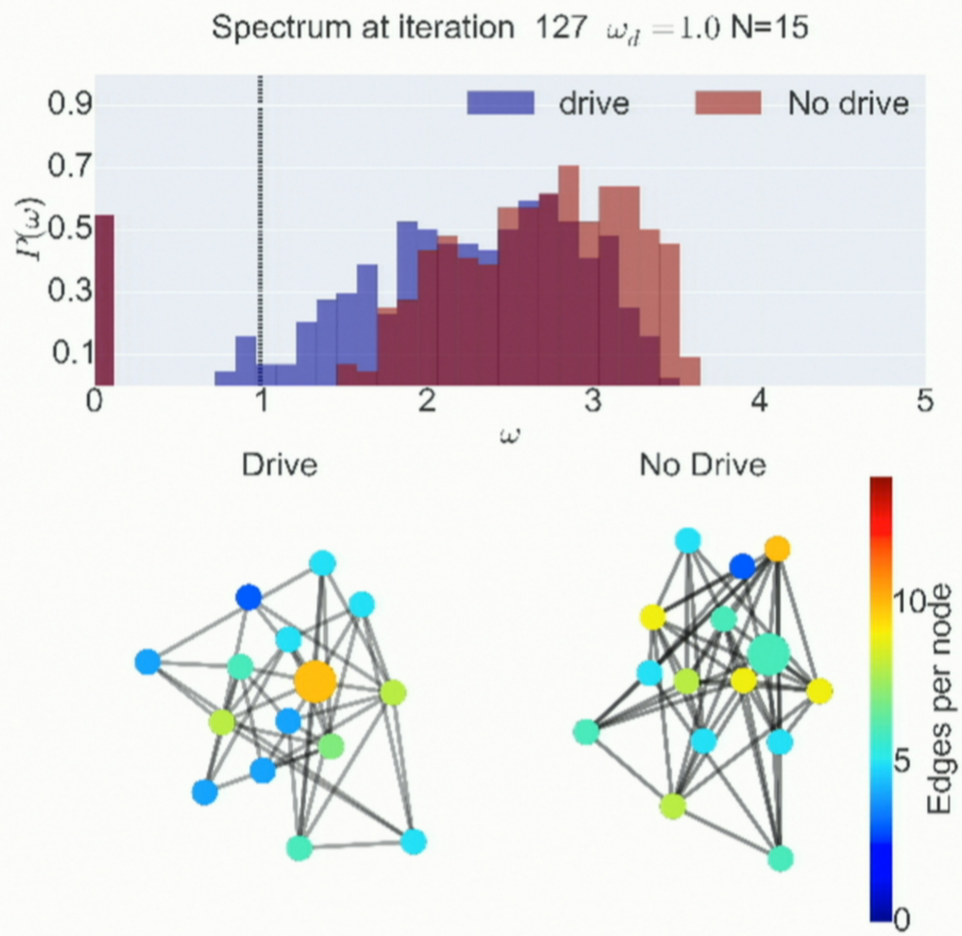
As time passes network resonates more with drive

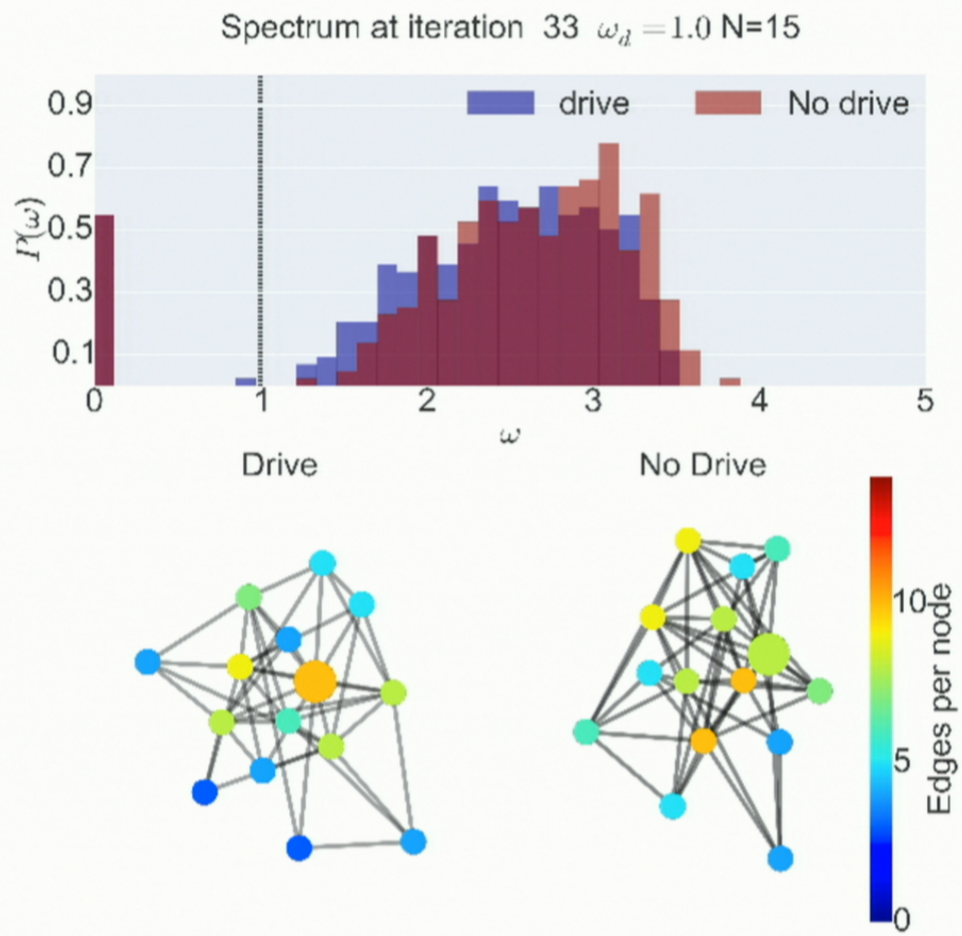


Springs rearrange to absorb more work from single driven particle




Spectrum at iteration 58 $\omega_d = 1.0$ N=15
drive
No drive
$P(\omega)$
0.9
0.7
0.5
0.3
0.1
0
1
2
3
4
5
ω
Drive
No Drive
Edges per node
10
5
0


Spectrum at iteration 127 $\omega_d = 1.0$ N=15
drive
No drive
$P(\omega)$
0.9
0.7
0.5
0.3
0.1
0
1
2
3
4
5
ω
Drive
No Drive
Edges per node
10
5
0

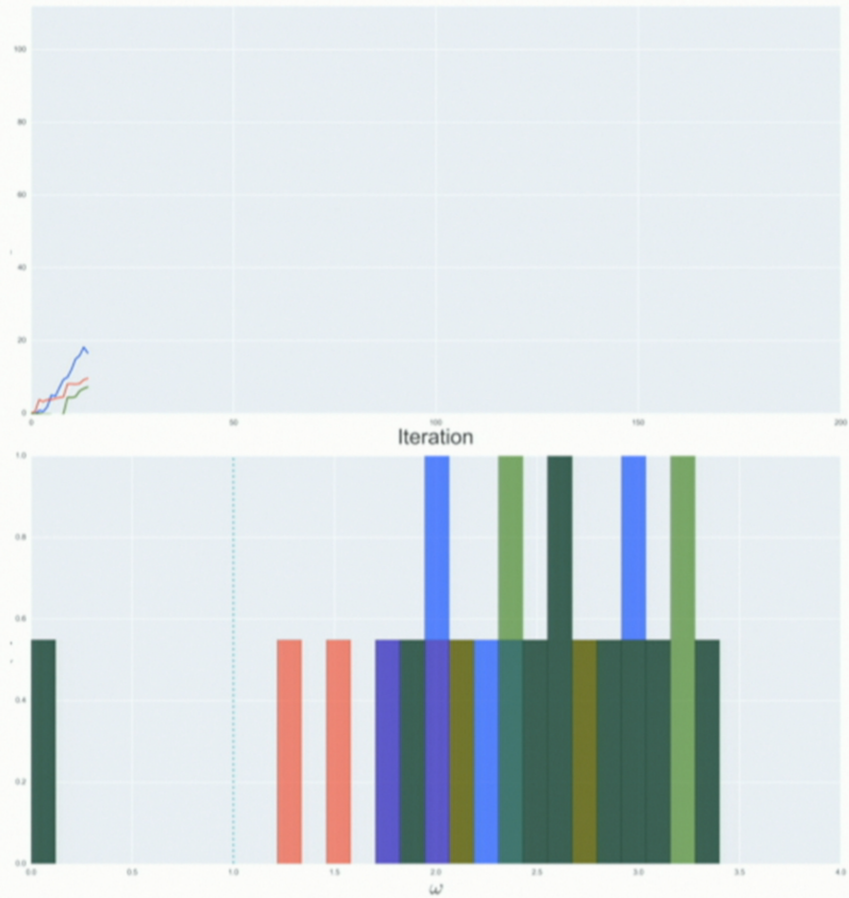


Spectrum at iteration 33 $\omega_d = 1.0$ N=15
drive
No drive
0.9
0.7
0.5
0.3
0.1
$P(\omega)$
0
1
2
3
4
5
ω
Drive
No Drive
10
5
0
Edges per node

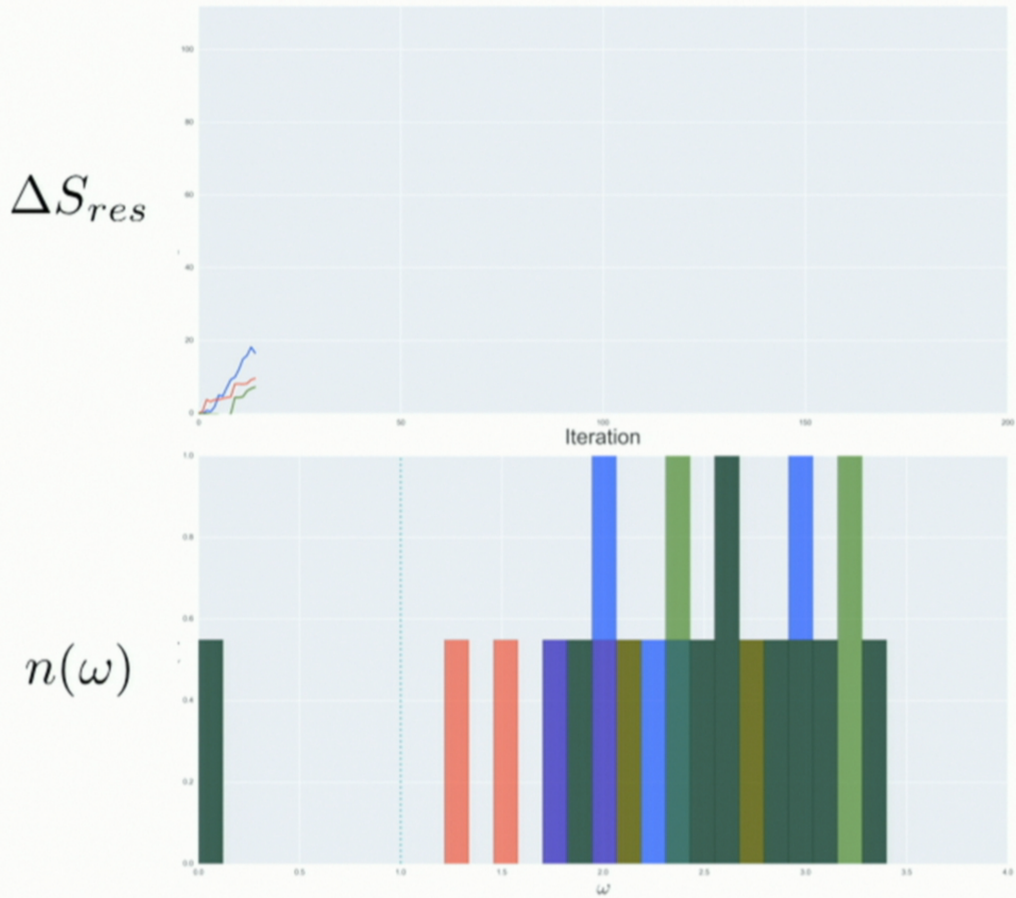
Entropy Production

ΔS_{res}

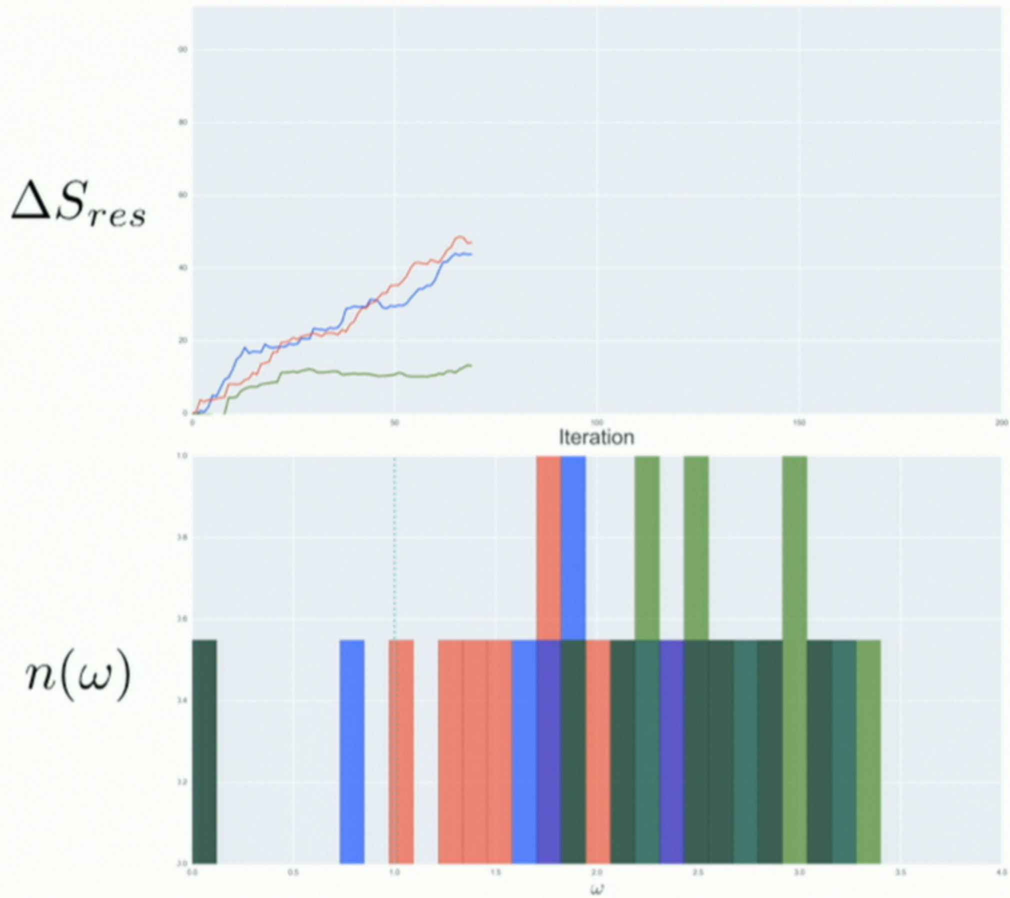
$n(\omega)$



Entropy Production



Entropy Production



Summary

Time-reversibility of Newton's Laws guarantees relationship between irreversibility and entropy production

Structures that form through reliable entropy production in a time-varying environment should seem adapted to 'eating'

We are able to demonstrate this 'learned' resonance by simulating a simple toy chemistry in an oscillating drive

Future Directions

Explaining some aspects of biological organization without Darwinian selection

Demonstrating more complex adaptation phenomena in driven ‘inanimate’ systems

Looking for signatures of sensing, prediction, and computation . . .

Thanks to . . .

Thomas and Virginia Cabot

Jeremy Owen
Cambridge U.

Tal Kachman
Technion

Robert Marsland
MIT