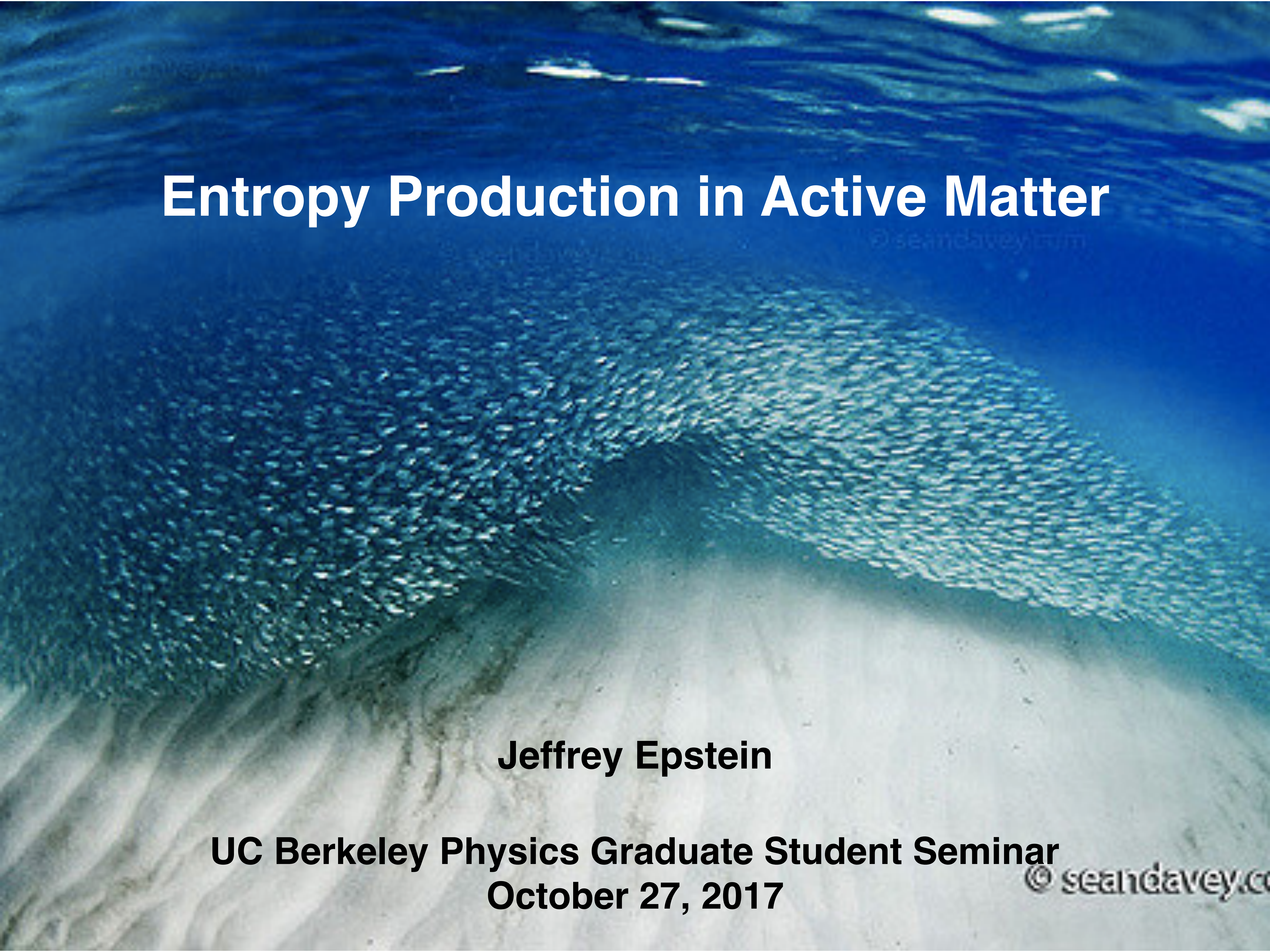
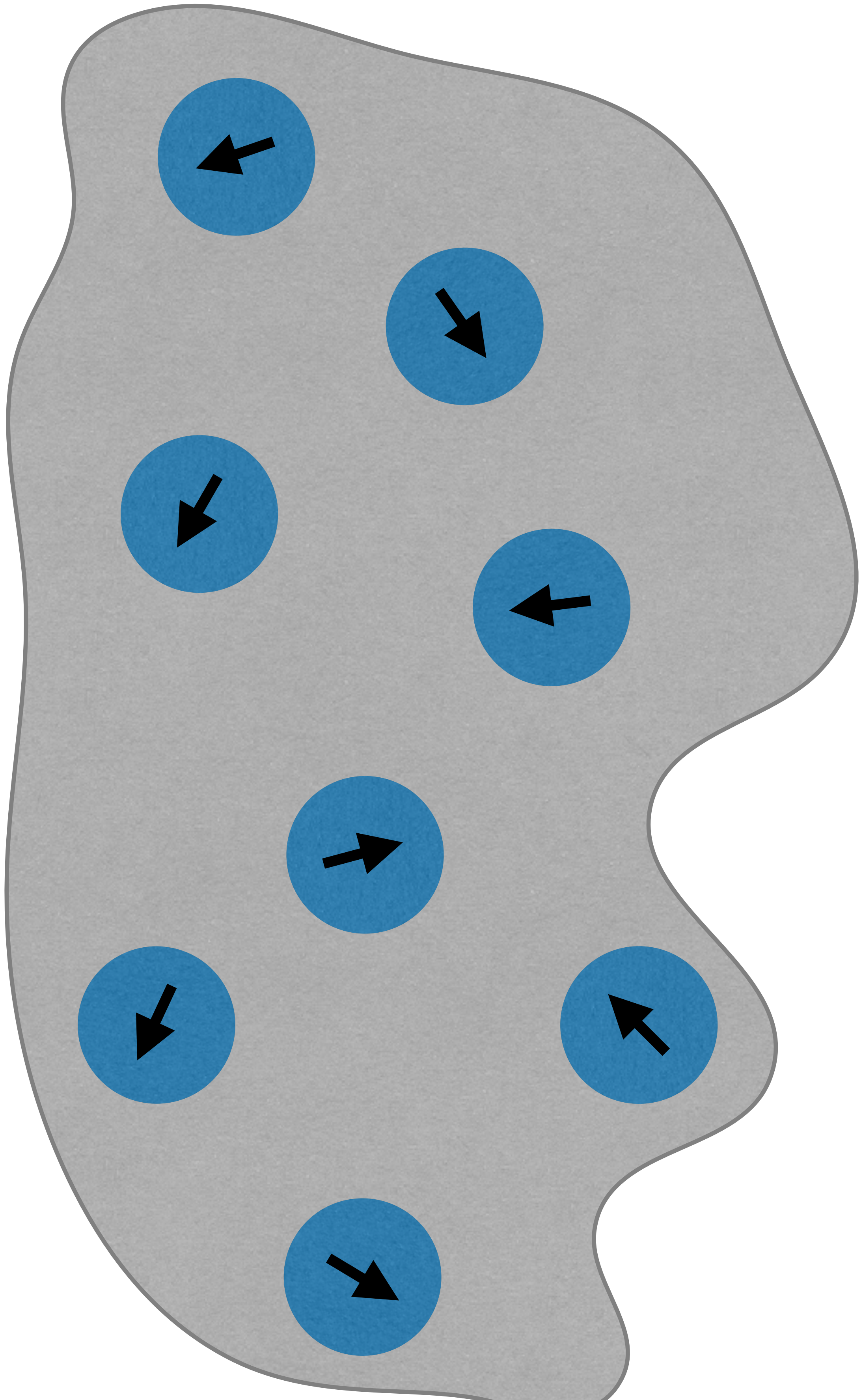


Entropy Production in Active Matter

Jeffrey Epstein

UC Berkeley Physics Graduate Student Seminar
October 27, 2017

Example: Motility-Induced Phase Separation (MIPS)



Microscopic Degrees of Freedom

Particle Positions $\mathbf{r}_k$

Particle Directors $\mathbf{e}_k$

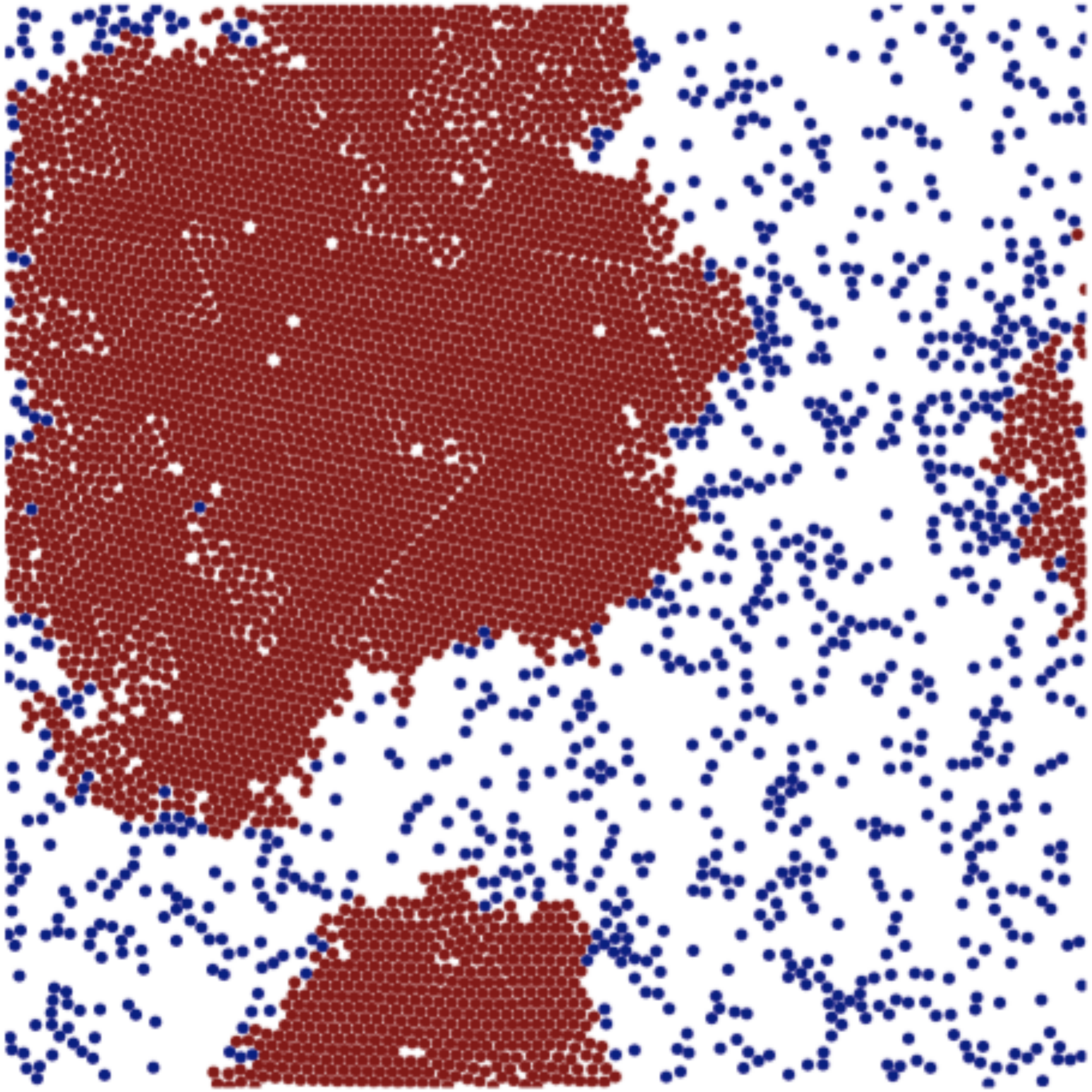
Microscopic Equations of Motion

$$\dot{\mathbf{r}}_k = -\nabla_k U + v\mathbf{e}_k + f_k$$

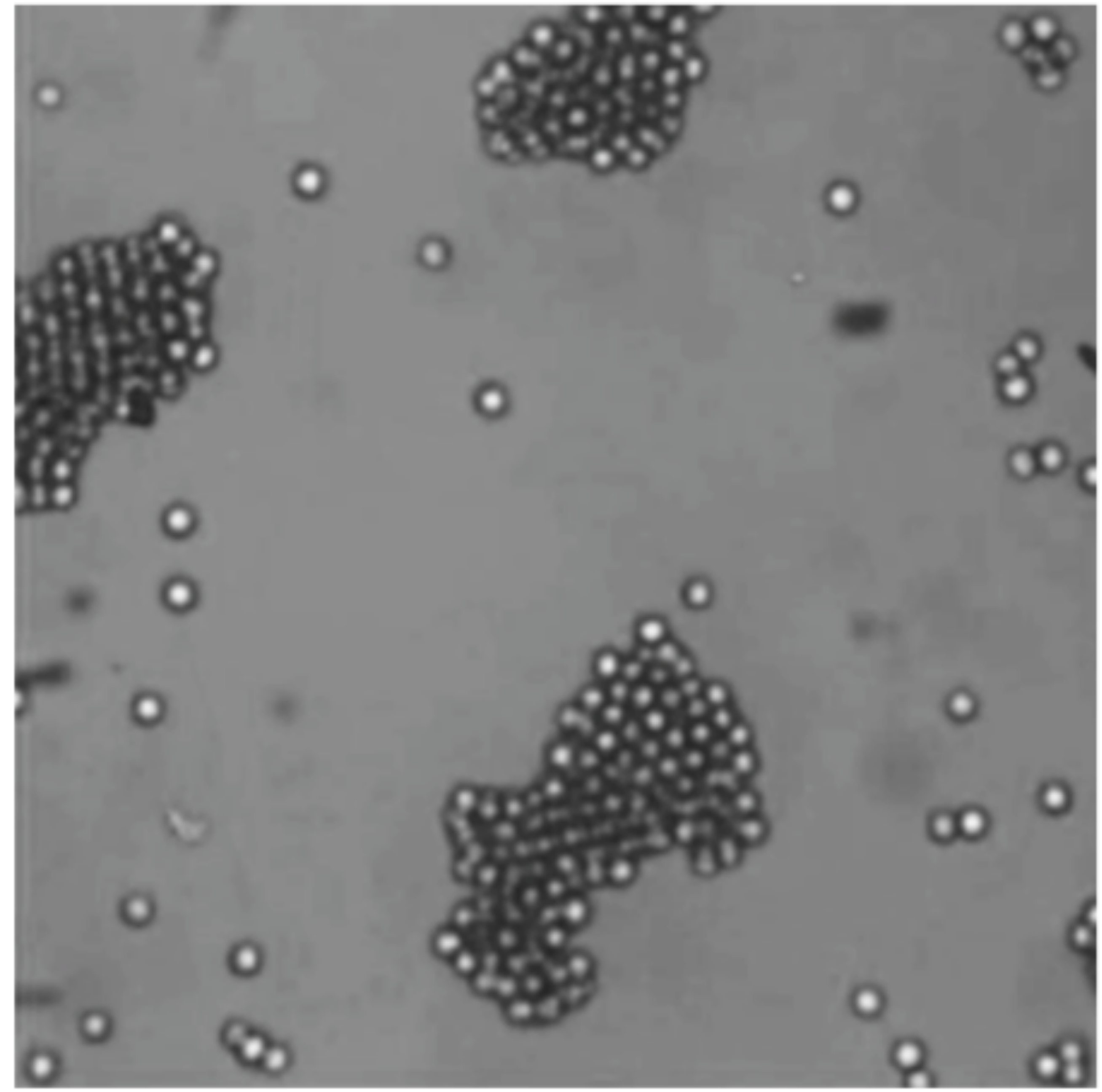
$$\dot{\mathbf{e}}_k = g_k$$

Buttinoni et al. PRL 2013

Example: Motility-Induced Phase Separation (MIPS)



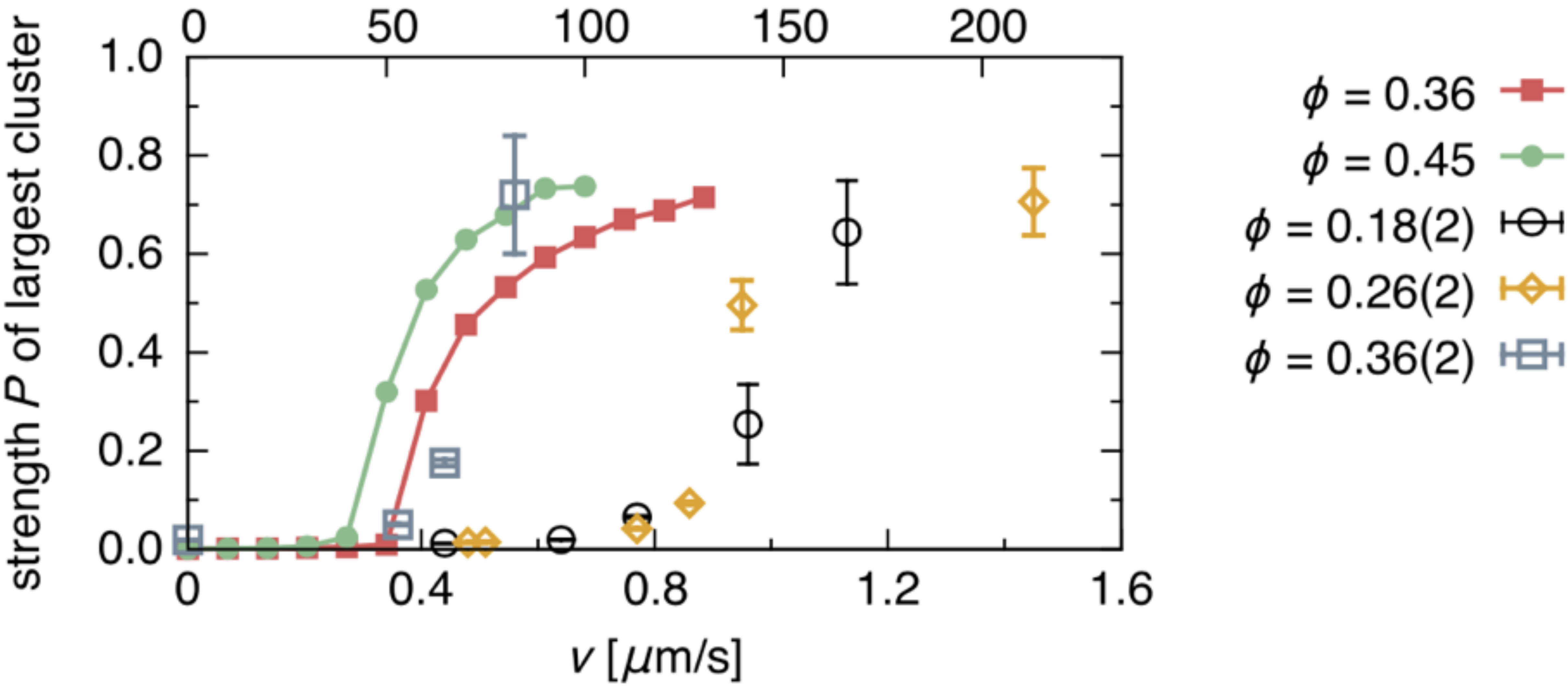
Simulation



Experiment

Buttinoni et al. PRL 2013

Example: Motility-Induced Phase Separation (MIPS)



Buttinoni et al. PRL 2013

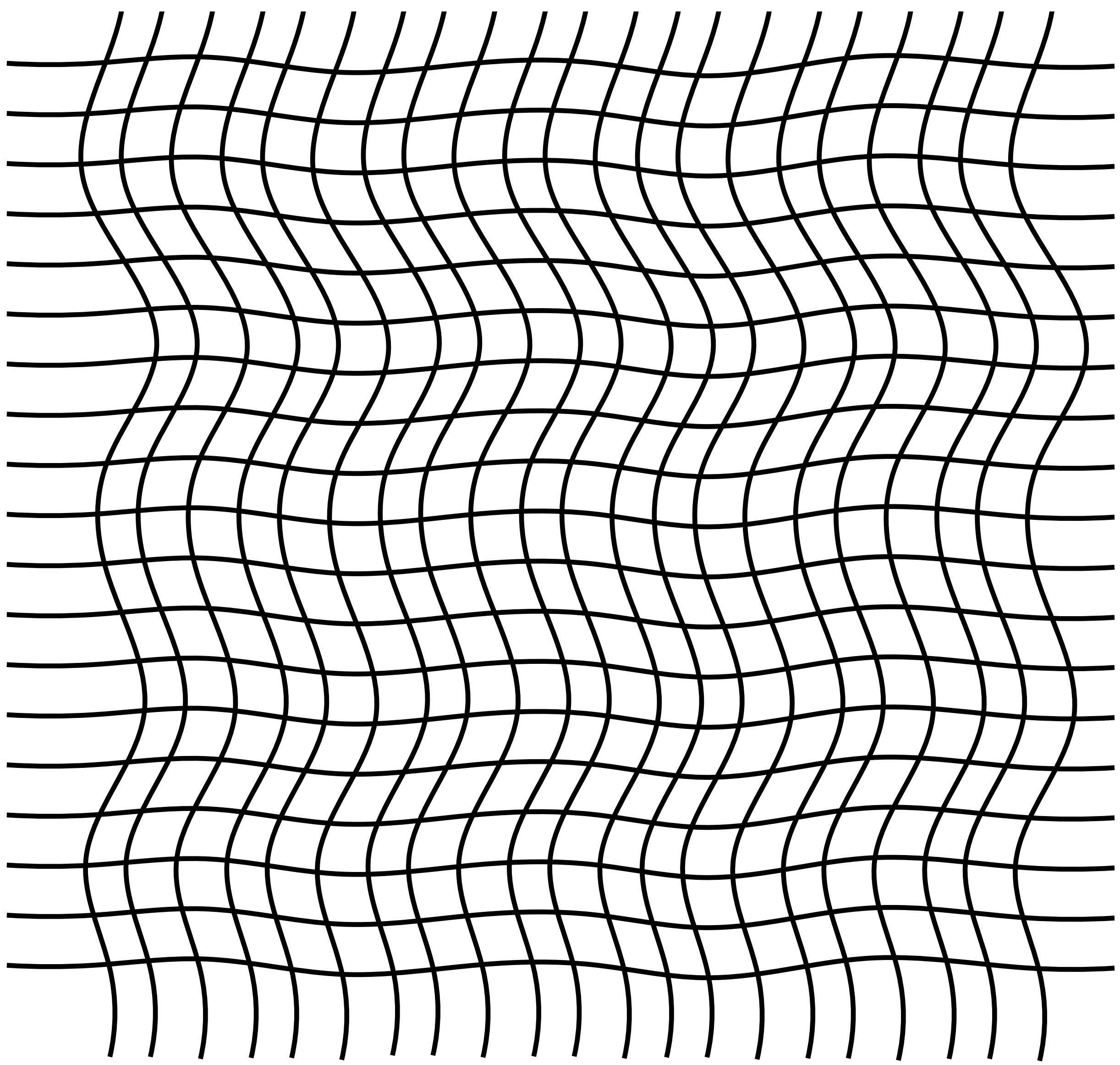
Example: Motility-Induced Phase Separation (MIPS)

Palacci et al. Science 2013

Why study entropy production in non-equilibrium systems?

Continuum Mechanics

$$\rho \frac{dv}{dt} = -\nabla p - \nabla \cdot \Pi$$

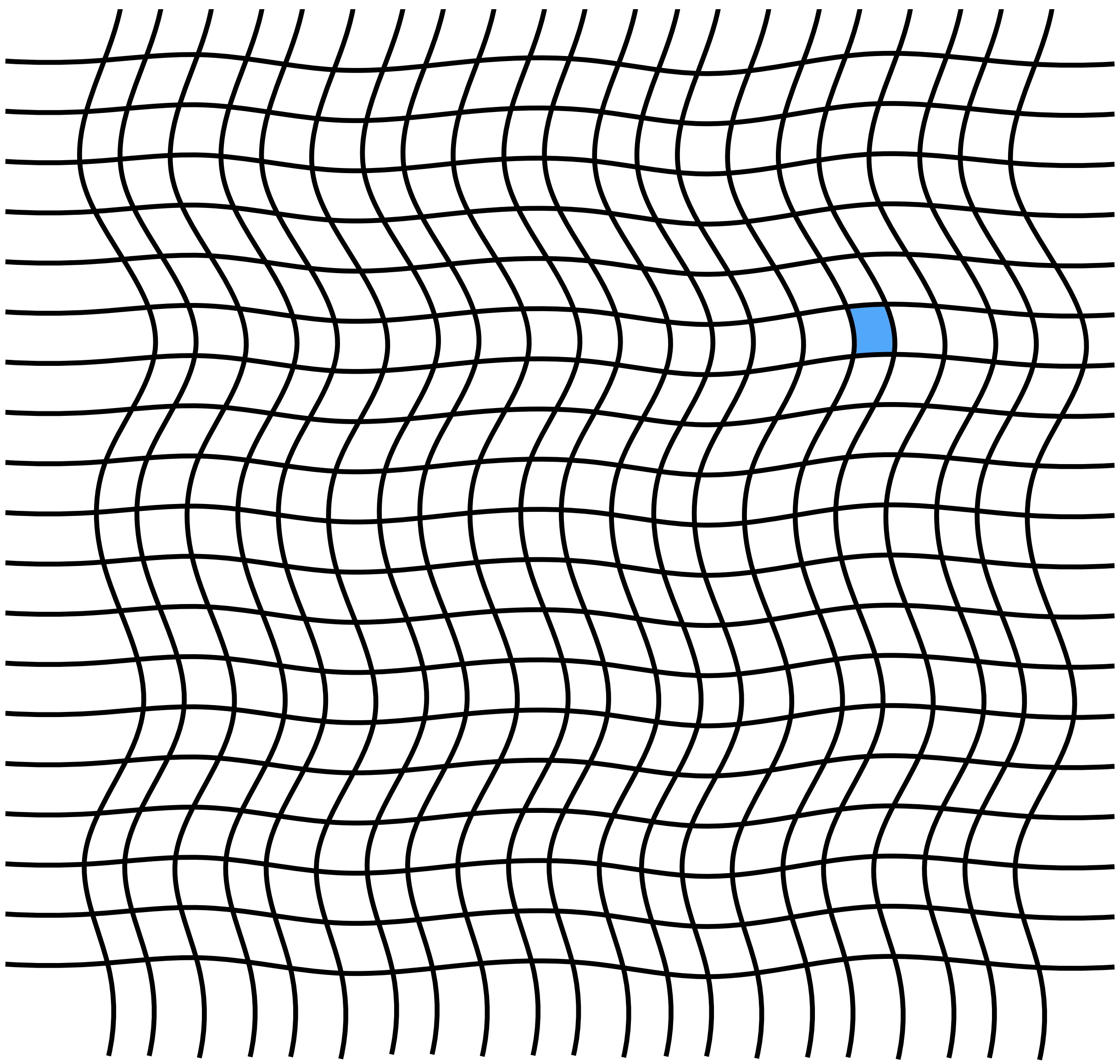


Rational Thermodynamics, C. Truesdell
Non-Equilibrium Thermodynamics, de Groot, Mazur

Why study entropy production in non-equilibrium systems?

Continuum Mechanics

$$\rho \frac{dv}{dt} = -\nabla p - \nabla \cdot \Pi$$

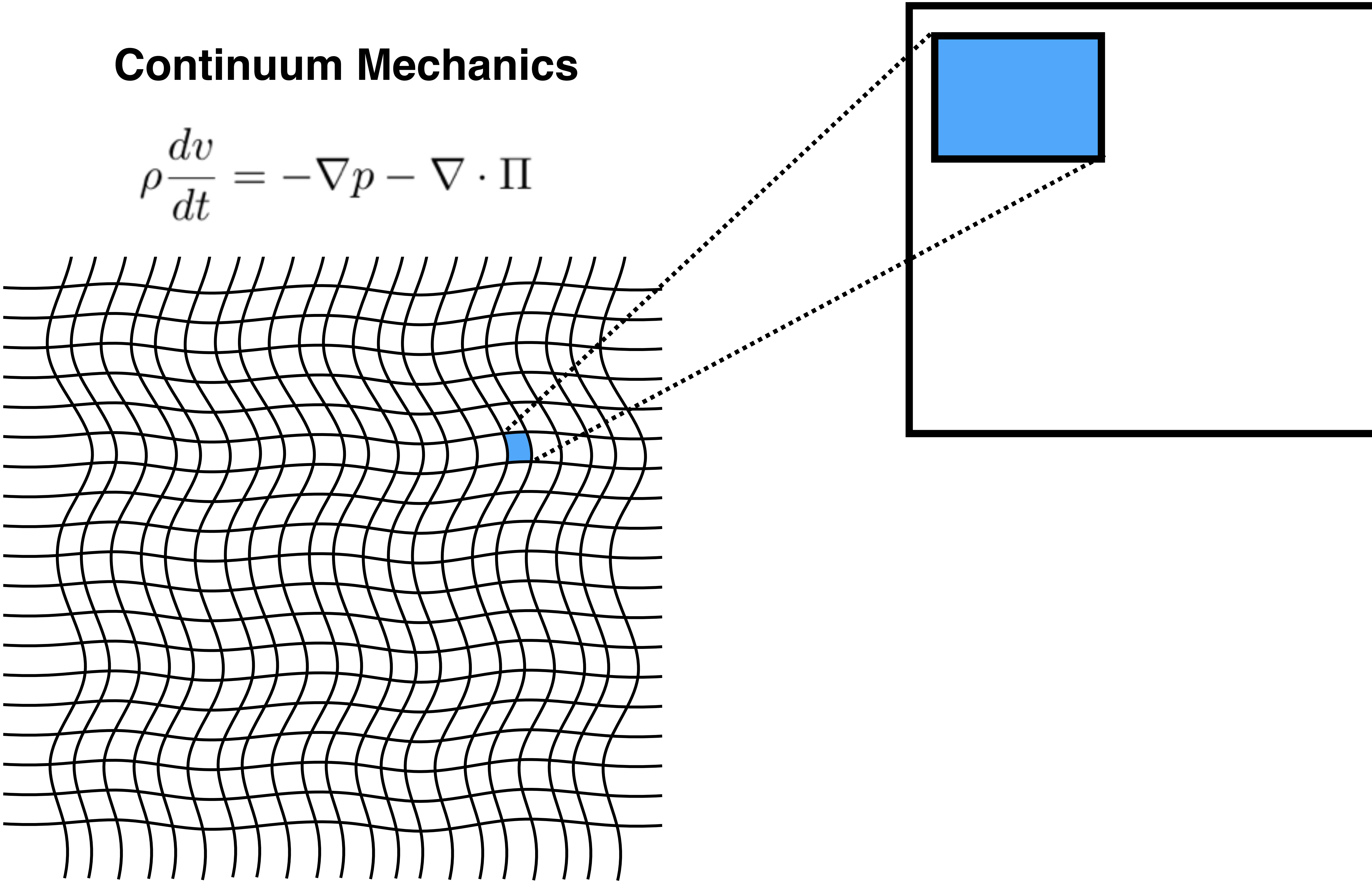


Rational Thermodynamics, C. Truesdell
Non-Equilibrium Thermodynamics, de Groot, Mazur

Why study entropy production in non-equilibrium systems?

Continuum Mechanics

$$\rho \frac{dv}{dt} = -\nabla p - \nabla \cdot \Pi$$

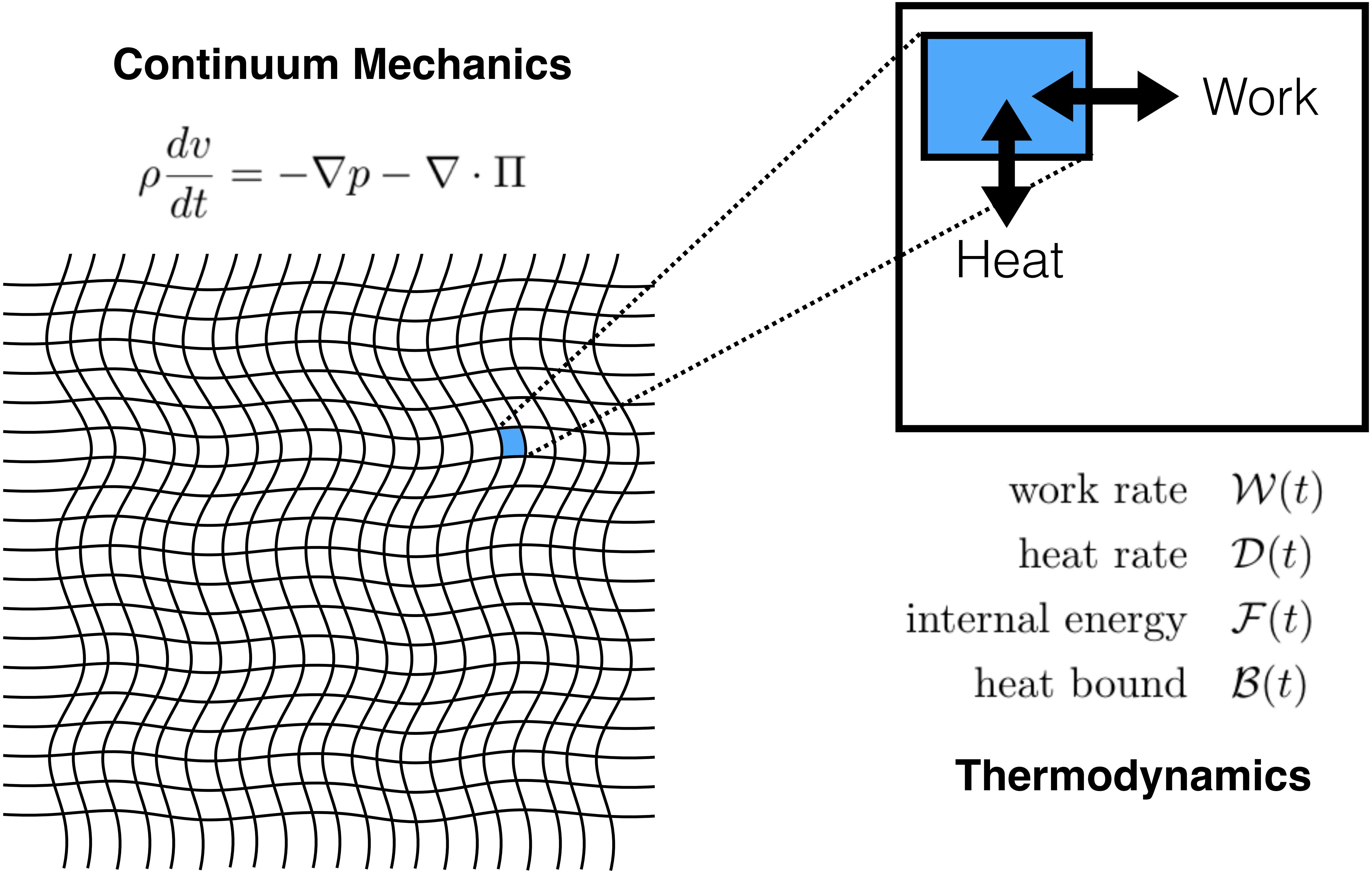


Rational Thermodynamics, C. Truesdell
Non-Equilibrium Thermodynamics, de Groot, Mazur

Why study entropy production in non-equilibrium systems?

Continuum Mechanics

$$\rho \frac{dv}{dt} = -\nabla p - \nabla \cdot \Pi$$



work rate	$\mathcal{W}(t)$
heat rate	$\mathcal{D}(t)$
internal energy	$\mathcal{F}(t)$
heat bound	$\mathcal{B}(t)$

Thermodynamics

Rational Thermodynamics, C. Truesdell
Non-Equilibrium Thermodynamics, de Groot, Mazur

Why study entropy production in non-equilibrium systems?

Heat is absorbed through boundaries

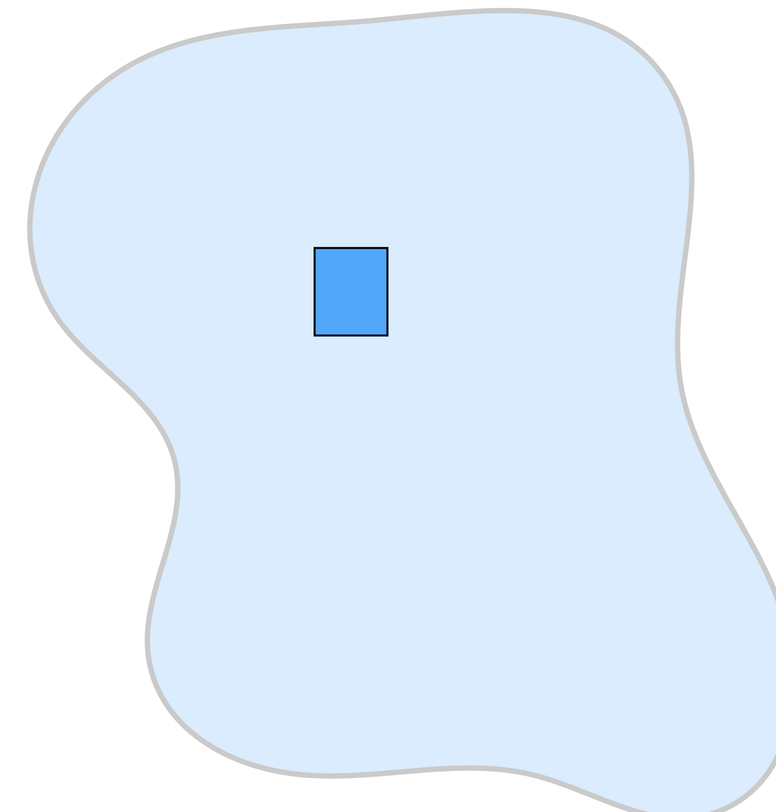
$$\mathcal{D}(t) = -\rho^{-1}\nabla \cdot J_q$$

Entropy has both a current and a source

$$\mathcal{B}(t) = \rho^{-1}T\left(-\nabla \cdot J_s + \sigma\right)$$

Work is defined within the mechanical theory

$$\mathcal{W}(t) = -p\frac{dJ}{dt} - \rho^{-1}\Pi : \nabla v$$



Non-Equilibrium Thermodynamics, de Groot, Mazur

Why study entropy production in non-equilibrium systems?

Heat is absorbed through boundaries

$$\mathcal{D}(t) = -\rho^{-1}\nabla \cdot J_q$$

Entropy has both a current and a source

$$\mathcal{B}(t) = \rho^{-1}T\left(-\nabla \cdot J_s + \sigma\right)$$

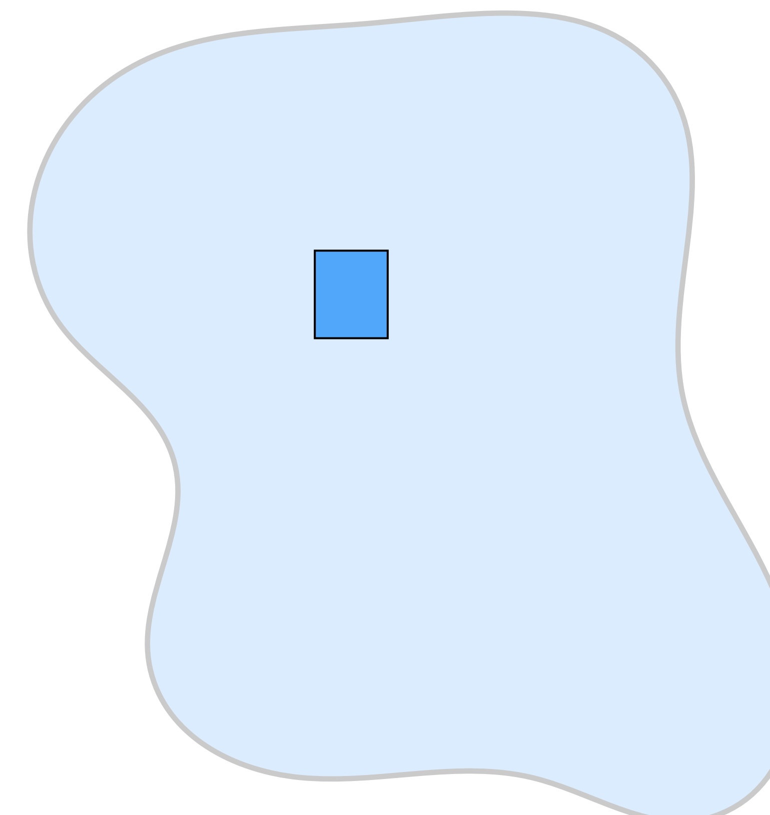
Work is defined within the mechanical theory

$$\mathcal{W}(t) = -p\frac{dJ}{dt} - \rho^{-1}\Pi : \nabla v$$

Assume Local equilibrium $\quad \mathcal{B}(t) = \dot{\mathcal{F}}(t) + p\dot{J}$

Assume entropy production takes the form

$$\boxed{\sigma = \sum_r J_r :: X_r \qquad J_r = \mathrm{lin}(\{X_q\})}$$



Non-Equilibrium Thermodynamics, de Groot, Mazur

Why study entropy production in non-equilibrium systems?

After some algebra…

$$\rho \frac{dv}{dt} = -\nabla p + \eta \triangle v + \left(\frac{1}{3} \eta + \eta_v \right) \nabla \left(\nabla \cdot v \right)$$

This is Navier-Stokes!

It's simple to add in temperature gradients and multiple reacting species.

Non-Equilibrium Thermodynamics, de Groot, Mazur

Why study entropy production in non-equilibrium systems?

After some algebra…

$$\rho \frac{dv}{dt} = -\nabla p + \eta \triangle v + \left(\frac{1}{3}\eta + \eta_v \right) \nabla \left(\nabla \cdot v \right)$$

This is Navier-Stokes!

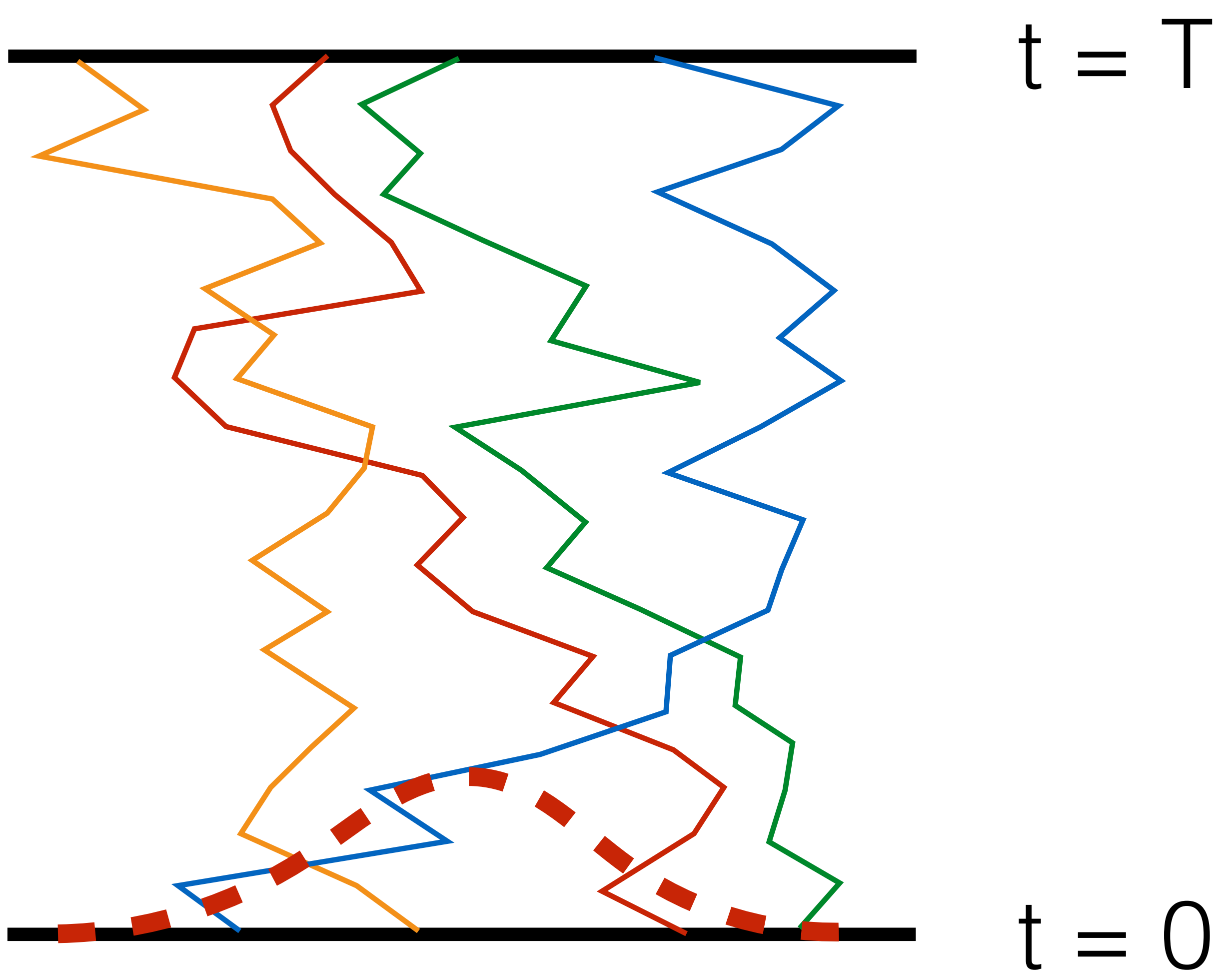
It's simple to add in temperature gradients and multiple reacting species.

Local Equilibrium
Continuum Mechanics → LIT Form of EP → Hydrodynamics

Non-Equilibrium Thermodynamics, de Groot, Mazur

What is entropy production? - Stochastic Thermodynamics

Goal: Associate thermodynamical quantities to individual trajectories.



$$\dot{x} = \mu F(x, \lambda) + \xi$$

$$\Pr\left[x(0) = x_0\right] = p(x_0)$$

$$p(\xi) = \frac{1}{2\sqrt{\pi D}} e^{-\xi^2/4D}$$

Can we quantify the “irreversibility” of a process?

What is entropy production? - Stochastic Thermodynamics

What is entropy production? - Stochastic Thermodynamics

Does a reversed trajectory generated by a reversed protocol look like a forwards trajectory?

What is entropy production? - Stochastic Thermodynamics

Does a reversed trajectory generated by a reversed protocol look like a forwards trajectory?

Define a protocol $F(x,t)$ and two probability distributions p and q on $\mathbb{R}$. Consider the following two samplers from the set of paths $x : [0,T] \to \mathbb{R}$:

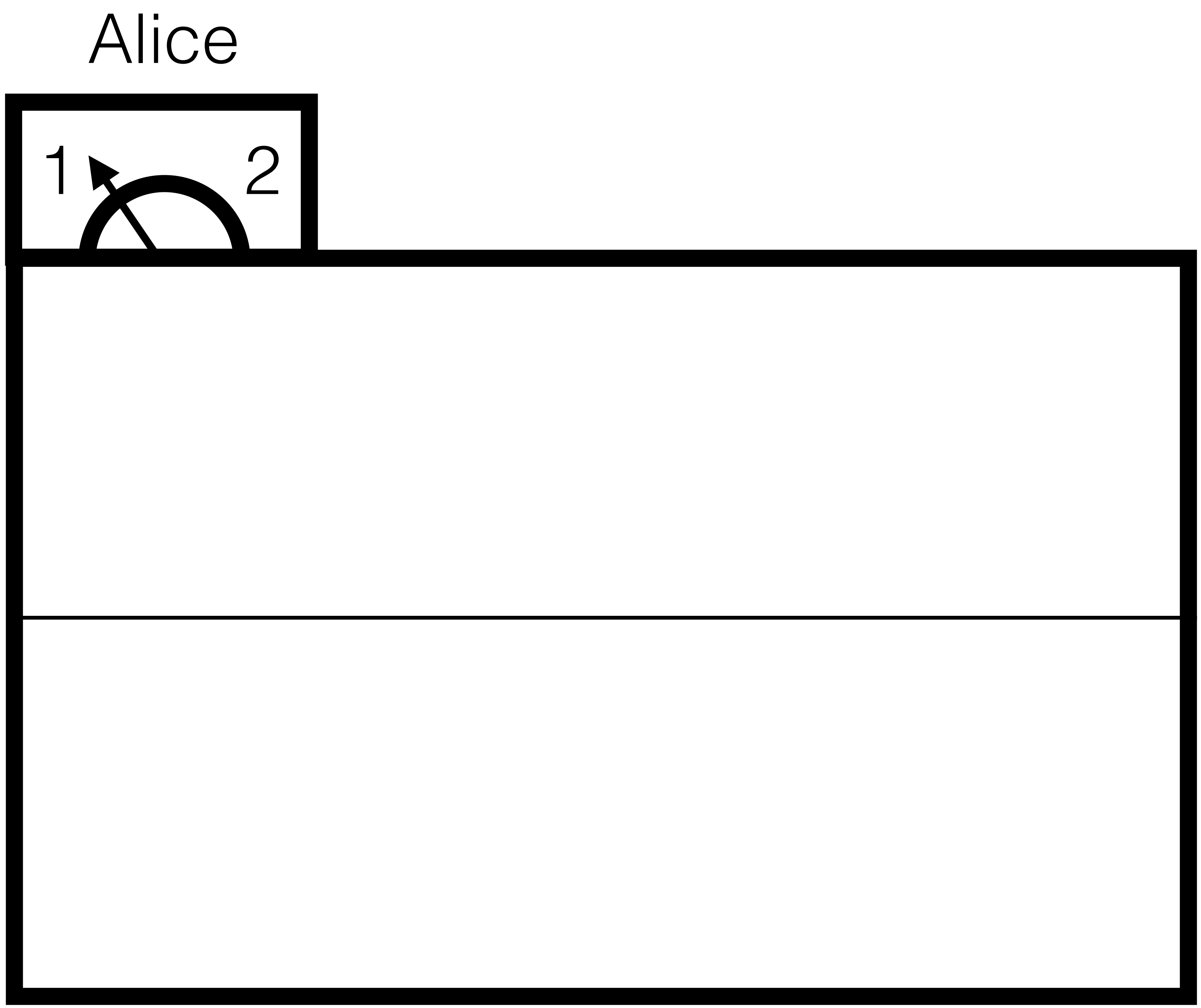
Sampler 1

1. Generate a point x_0 from the distribution p.
2. Generate a path $x : [0,T] \to \mathbb{R}$ with SDE $\dot{x}(t) = \mu F(x(t),t) + \xi(t)$ with initial condition $x(0) = x_0$.
3. Return x.

Sampler 2

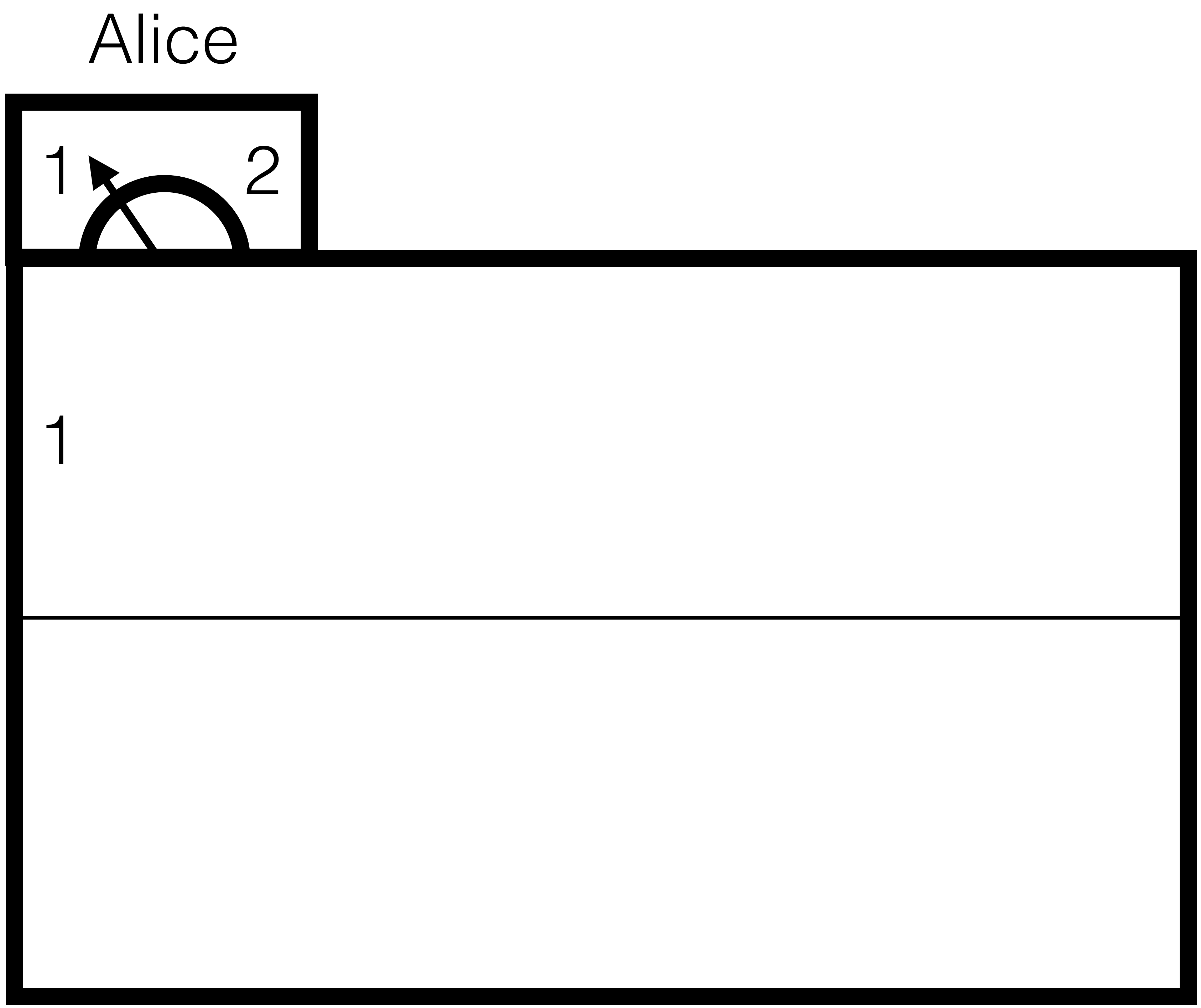
1. Generate a point y_0 from the distribution q.
2. Generate path $y : [0,T] \to \mathbb{R}$ with SDE $\dot{y}(t) = \mu F(y(t), T-t) + \xi(t)$ with initial condition $y(0) = y_0$.
3. Define $x(t) = y(T-t)$.
4. Return x.

What is entropy production? - Stochastic Thermodynamics



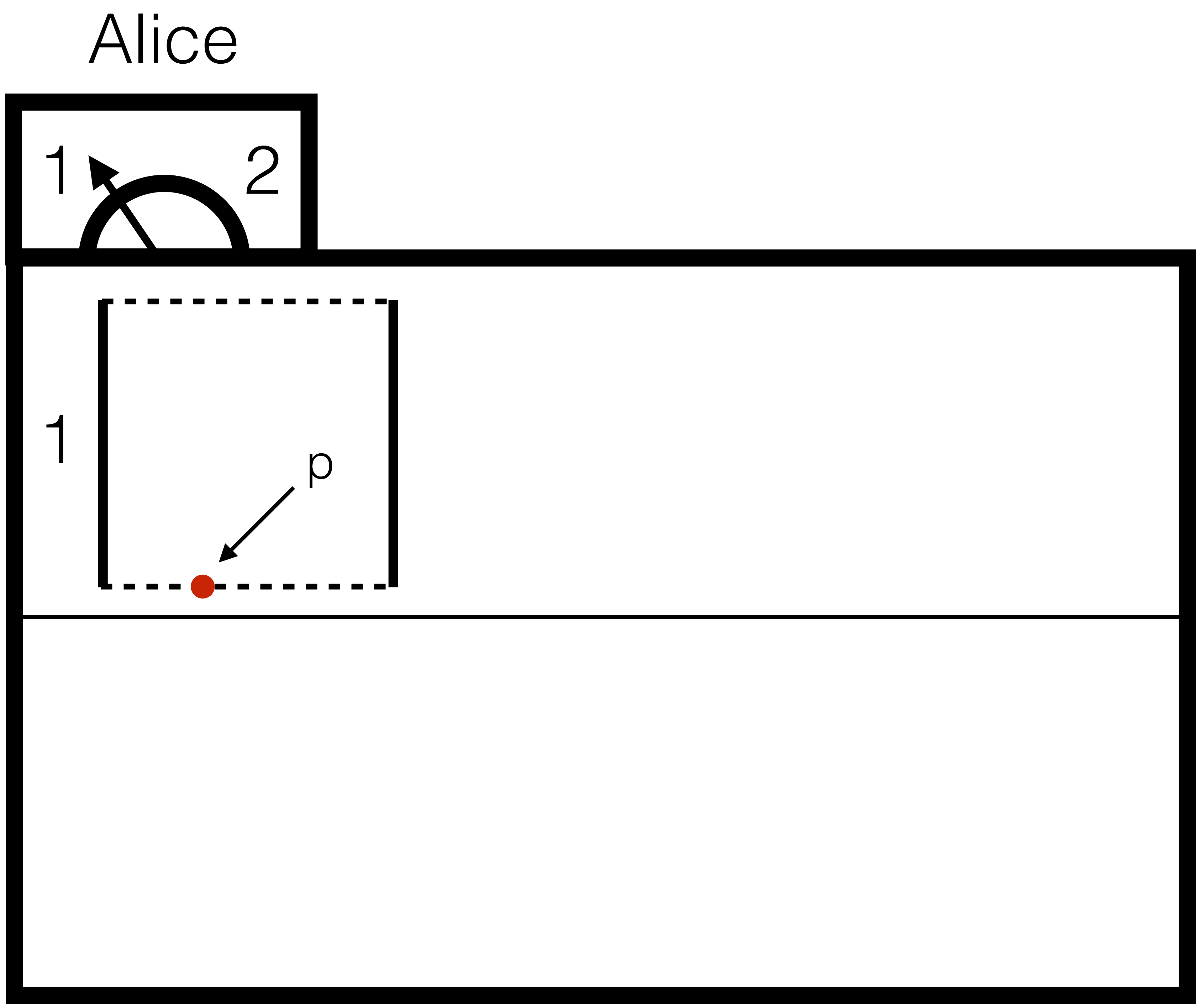
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



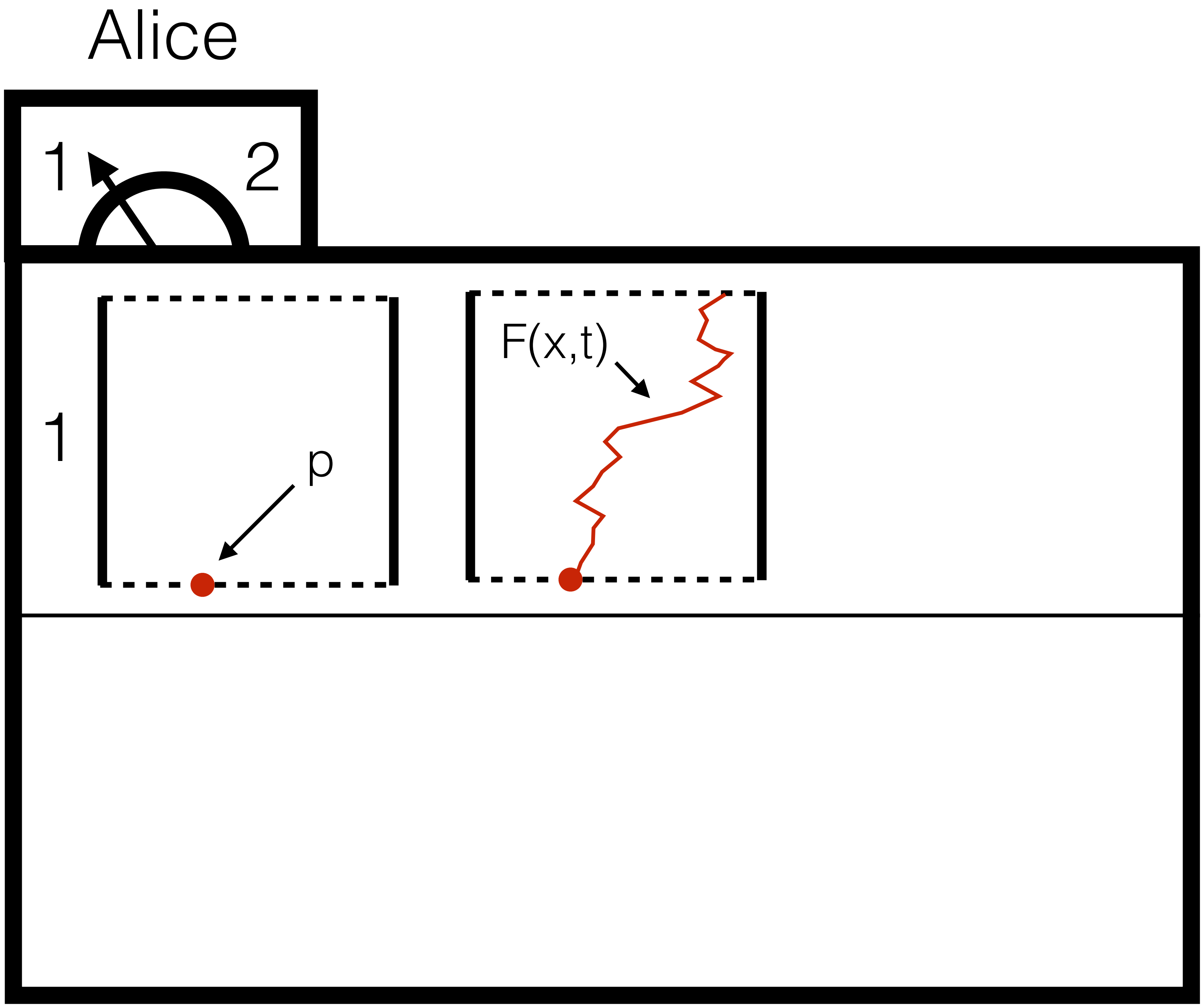
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



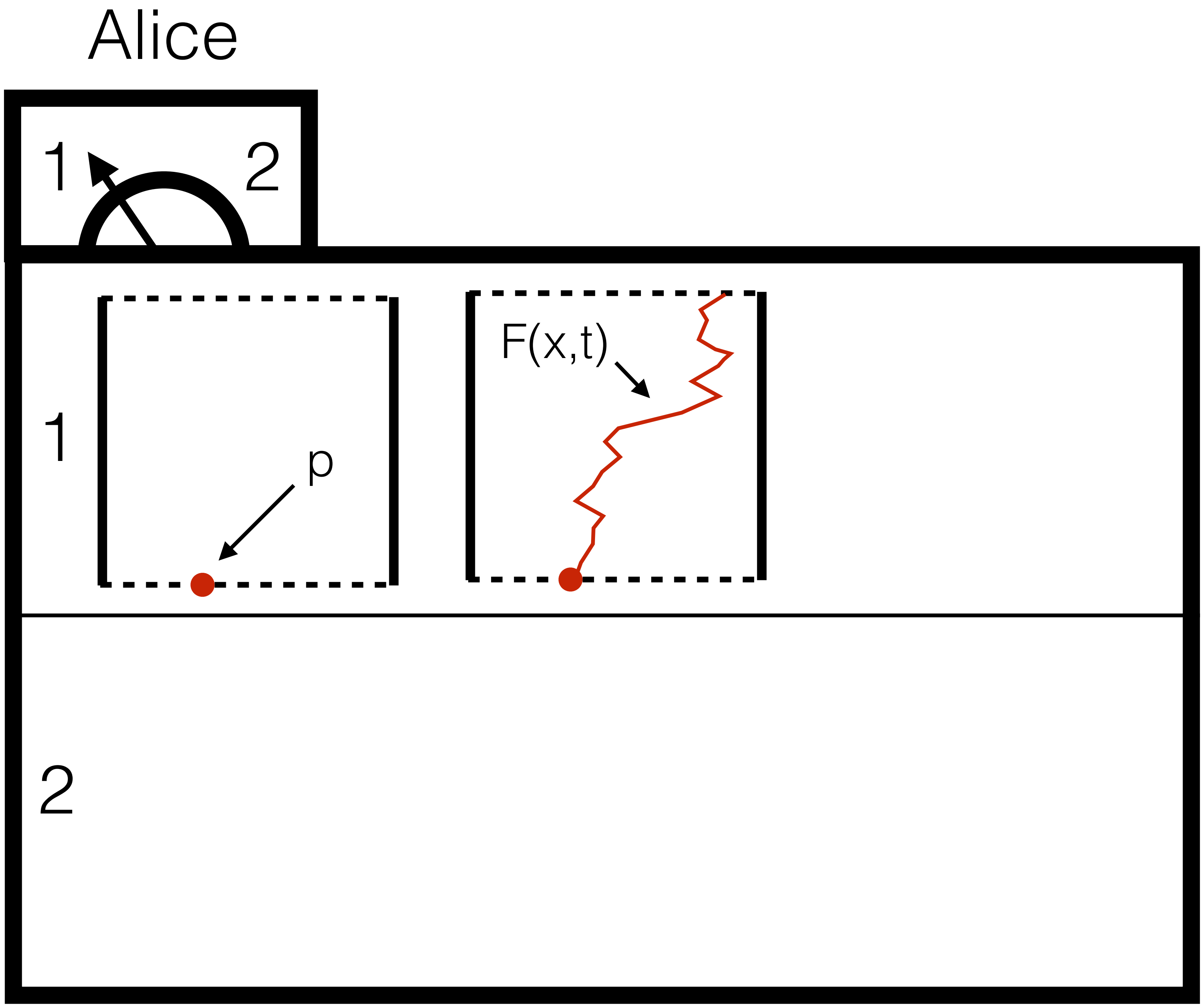
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



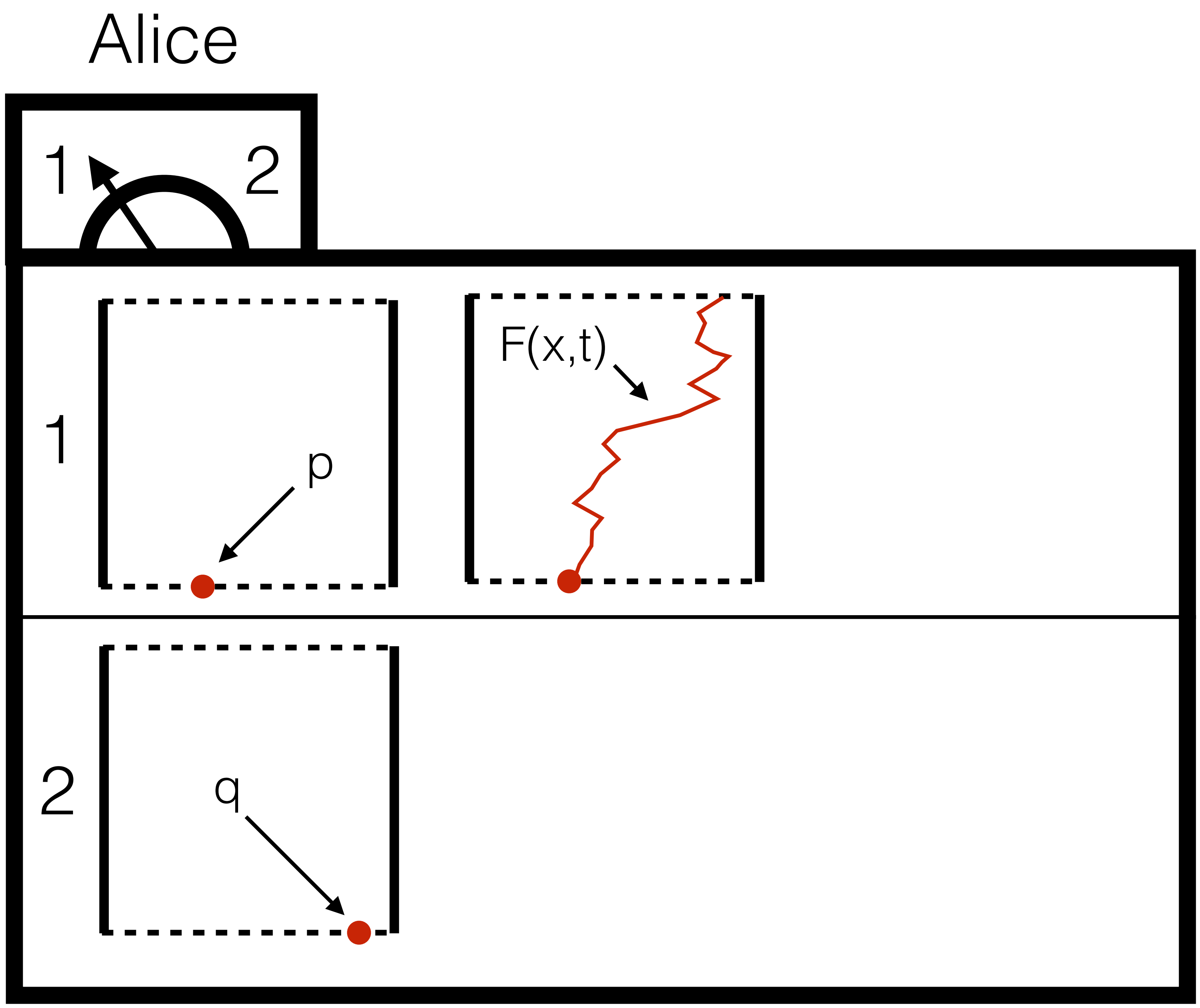
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



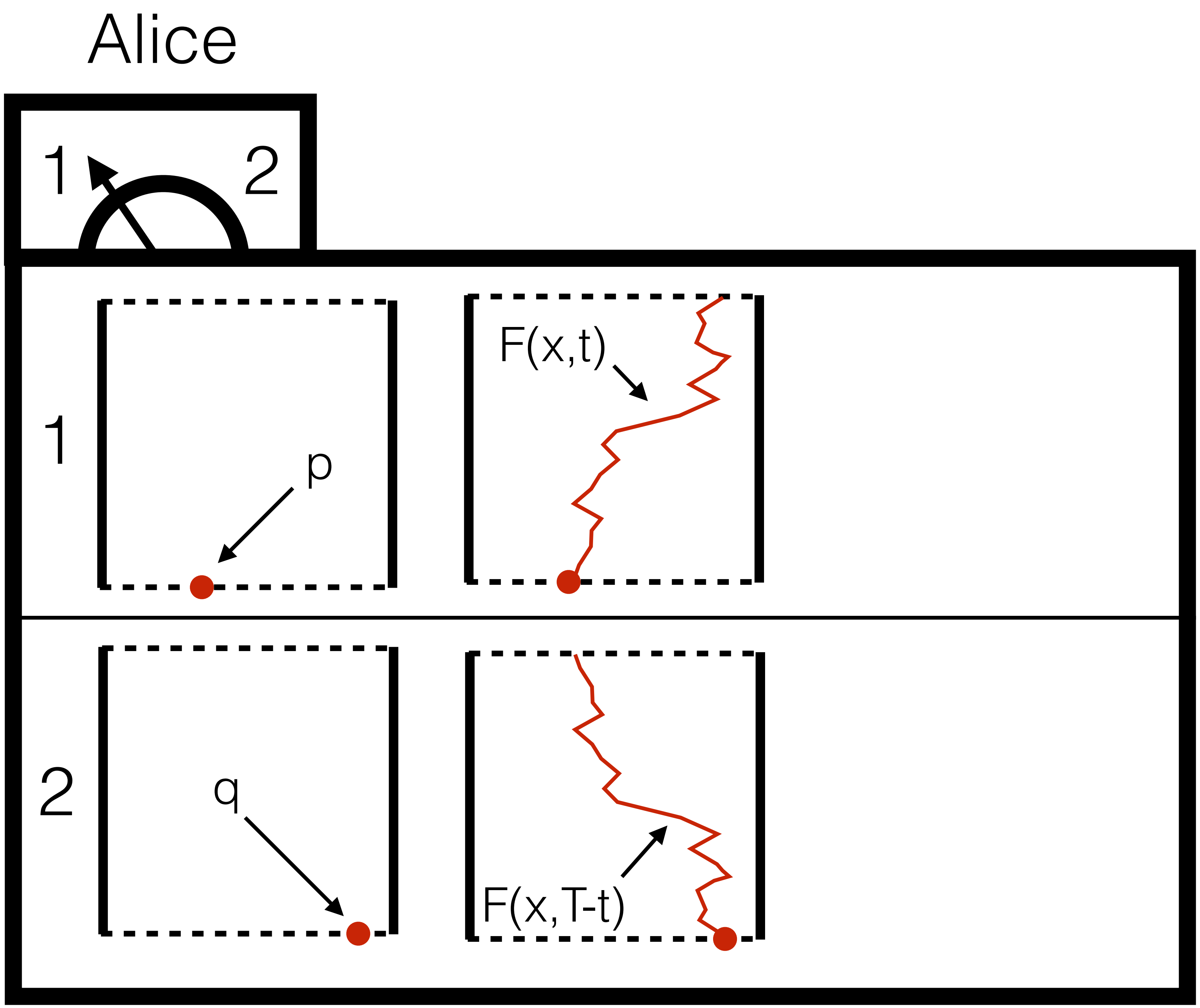
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



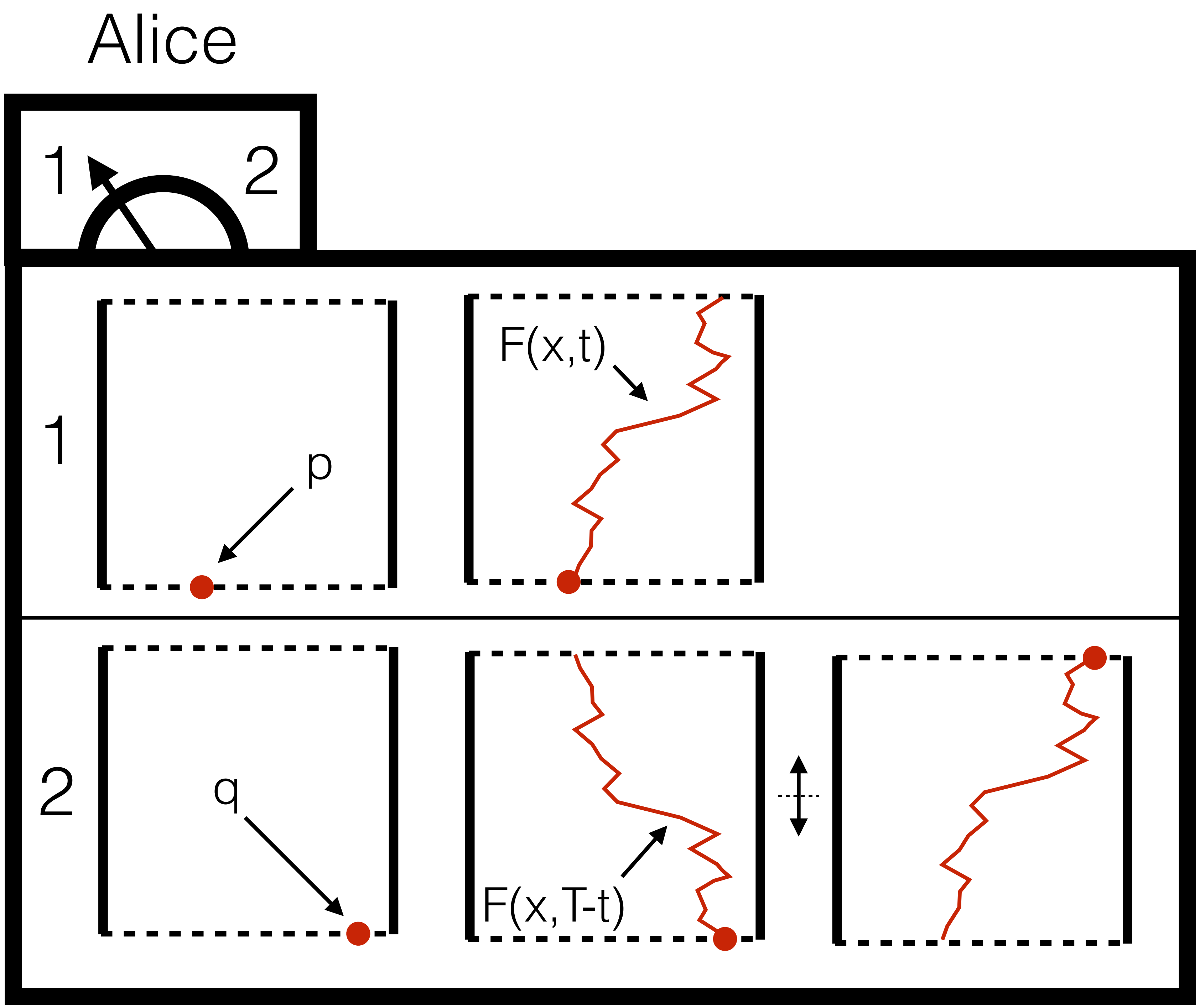
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



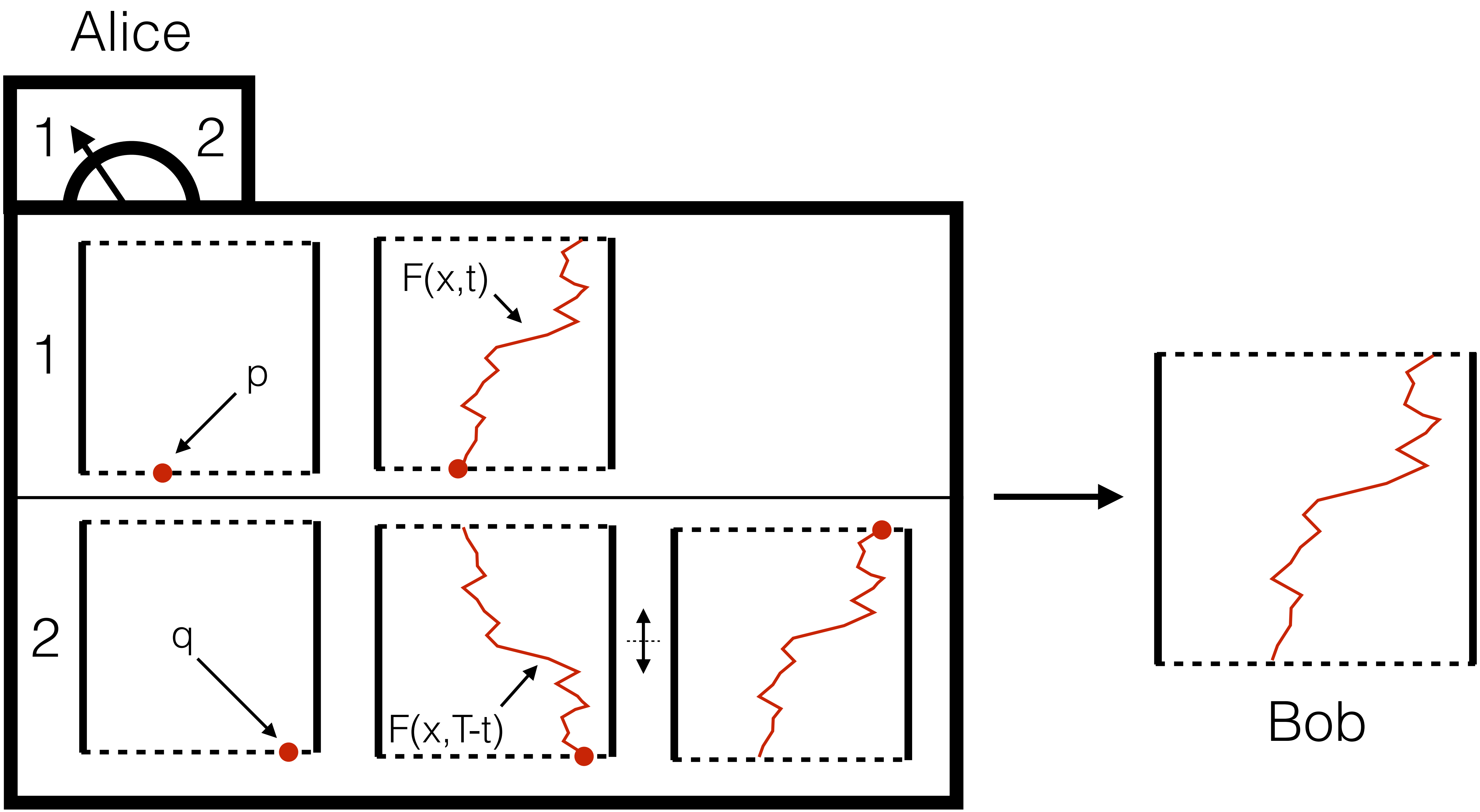
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



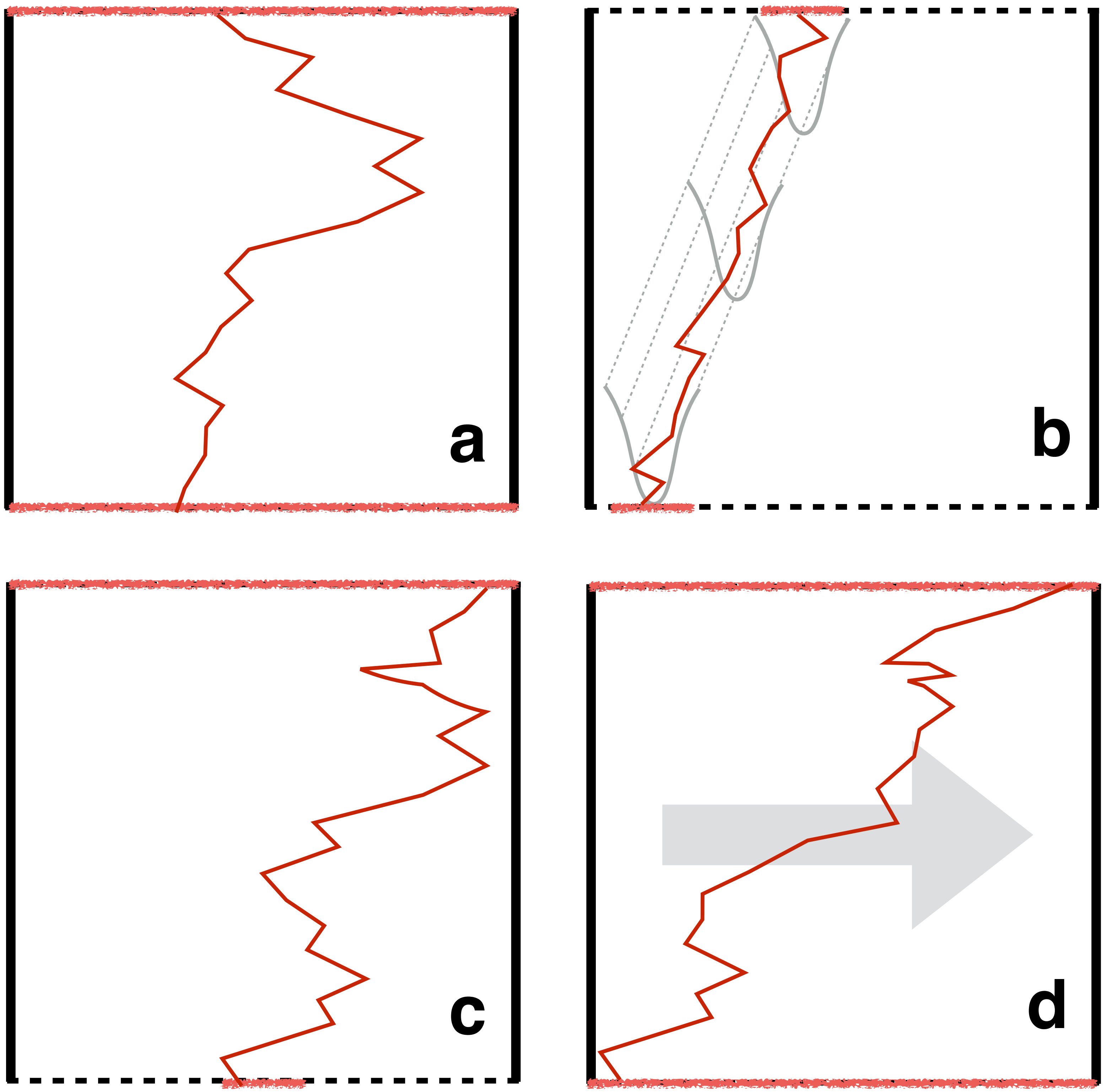
Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



Alice picks 1 or 2. Bob has to figure out which one.

What is entropy production? - Stochastic Thermodynamics



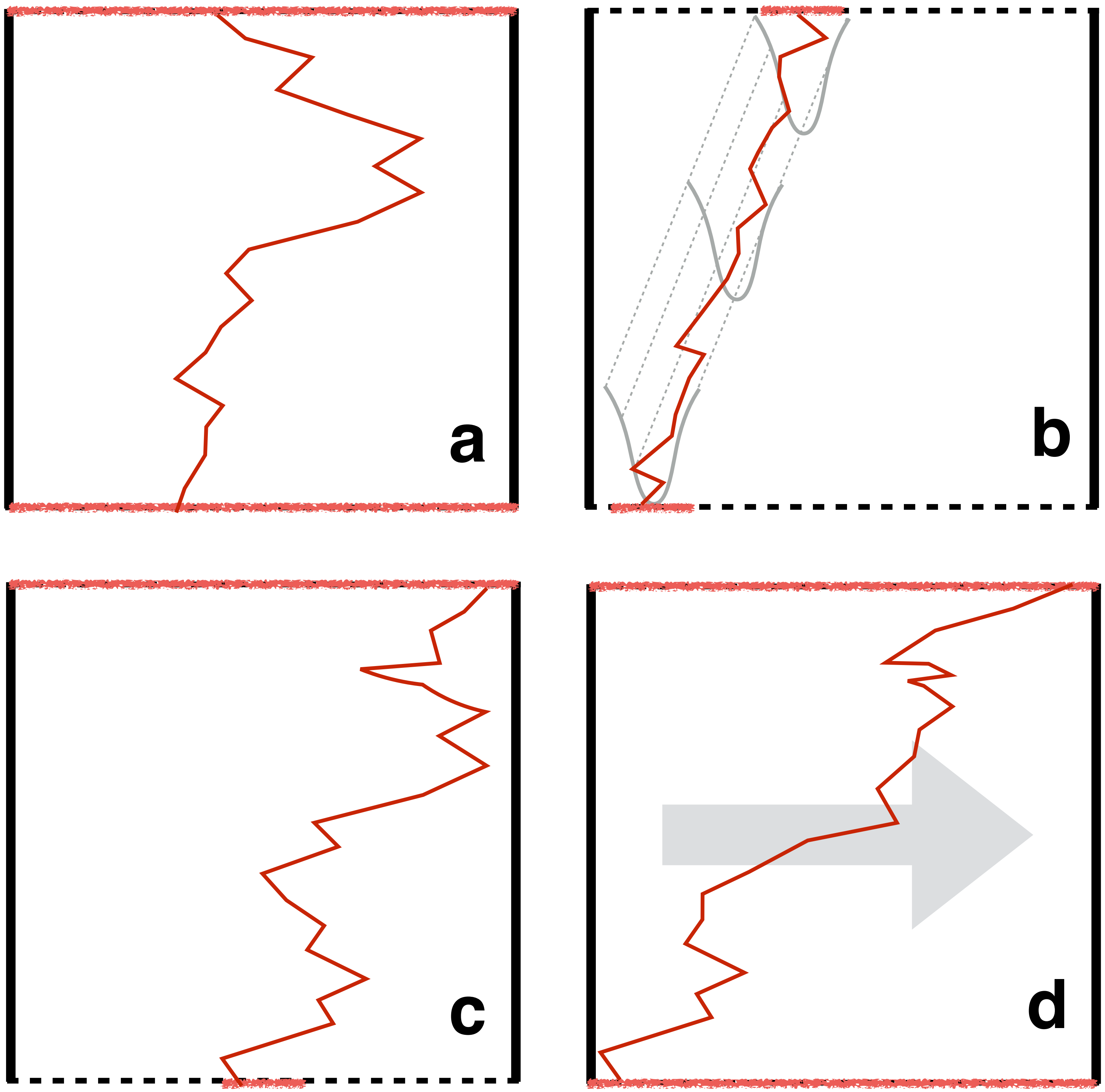
(a) Equilibrium

(b) Adiabatic Protocol

(c) Equilibration

(d) NESS

What is entropy production? - Stochastic Thermodynamics



(a) Equilibrium

(b) Adiabatic Protocol

(c) Equilibration

(d) NESS

Two modes of entropy production

What is entropy production? - Stochastic Thermodynamics

$$\Pr\left[\xi_x|1\right] \sim p(x(0)) \cdot \exp\left[-\int_0^T \frac{\xi_x(t)^2}{4D} dt\right] = p(x(0)) \cdot \exp\left[-\int_0^T \frac{\left(\dot{x}(t) - \mu F(x(t),t)\right)^2}{4D} dt\right]$$

$$\Pr\left[\xi_x|2\right] \sim q(x(t)) \cdot \exp\left[-\int_0^T \frac{\left(-\dot{x}(T-t) - \mu F(x(T-t), T-t\right)^2}{4D} dt\right]$$

What is entropy production? - Stochastic Thermodynamics

$$\Pr\left[\xi_x|1\right] \sim p(x(0)) \cdot \exp\left[-\int_0^T \frac{\xi_x(t)^2}{4D} dt\right] = p(x(0)) \cdot \exp\left[-\int_0^T \frac{\left(\dot{x}(t) - \mu F(x(t),t)\right)^2}{4D} dt\right]$$

$$\Pr\left[\xi_x|2\right] \sim q(x(t)) \cdot \exp\left[-\int_0^T \frac{\left(-\dot{x}(T-t) - \mu F(x(T-t), T-t\right)^2}{4D} dt\right]$$

$$\ln\left[\frac{\Pr\left[\xi_x|1\right]}{\Pr\left[\xi_x|1\right]}\right] = \ln\left[\frac{p(x(0))}{q(x(t))}\right] + \frac{\mu}{D}\int_0^T F(x(t),t)\dot{x}(t) dt$$

What is entropy production? - Stochastic Thermodynamics

$$\Pr\left[\xi_x|1\right] \sim p(x(0))\cdot\exp\left[-\int_0^T \frac{\xi_x(t)^2}{4D}dt\right] = p(x(0))\cdot\exp\left[-\int_0^T \frac{\left(\dot{x}(t)-\mu F(x(t),t)\right)^2}{4D}dt\right]$$

$$\Pr\left[\xi_x|2\right] \sim q(x(t))\cdot\exp\left[-\int_0^T \frac{\left(-\dot{x}(T-t)-\mu F(x(T-t),T-t\right)^2}{4D}dt\right]$$

$$\ln\left[\frac{\Pr\left[\xi_x|1\right]}{\Pr\left[\xi_x|1\right]}\right] = \ln\left[\frac{p(x(0))}{q(x(t))}\right] + \frac{\mu}{D}\int_0^T F(x(t),t)\dot{x}(t)dt$$

Work given to disordered degrees of freedom = heat

What is entropy production? - Stochastic Thermodynamics

$$\Pr\left[\xi_x|1\right] \sim p(x(0)) \cdot \exp\left[-\int_0^T \frac{\xi_x(t)^2}{4D} dt\right] = p(x(0)) \cdot \exp\left[-\int_0^T \frac{(\dot{x}(t) - \mu F(x(t),t))^2}{4D} dt\right]$$

$$\Pr\left[\xi_x|2\right] \sim q(x(t)) \cdot \exp\left[-\int_0^T \frac{(-\dot{x}(T-t) - \mu F(x(T-t), T-t)^2}{4D} dt\right]$$

$$\ln\left[\frac{\Pr\left[\xi_x|1\right]}{\Pr\left[\xi_x|1\right]}\right] = \ln\left[\frac{p(x(0))}{q(x(t))}\right] + \frac{\mu}{D}\int_0^T F(x(t),t)\dot{x}(t)dt$$

Work given to disordered degrees of freedom = heat

In steady-state with bath at T:

$$\Delta S = \frac{Q}{T}$$

To Do:

Actually compute entropy production for active matter systems and use a local steady-state hypothesis to derive hydrodynamics.

Understand how microscopic irreversibility gets reflected at the macroscale.


Thanks!
http://www.uwphotographyguide.com/akule-school-captured-kona