Nonequilibrium thermodynamics for active matter

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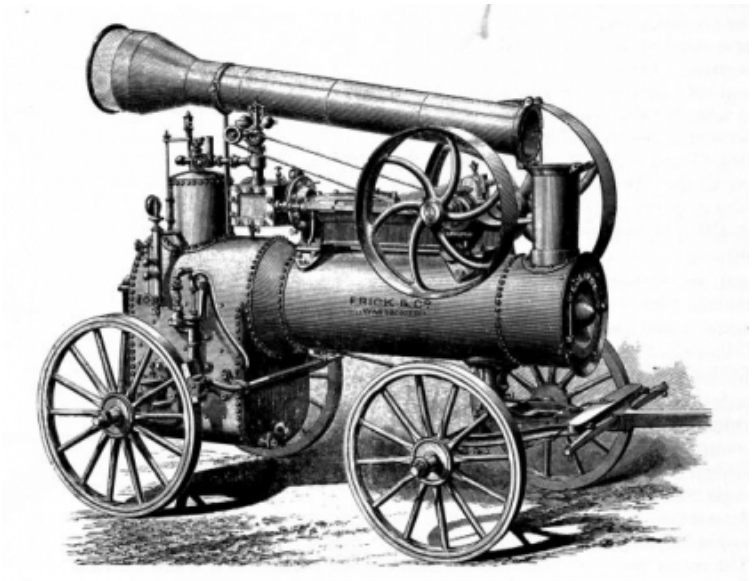
Active20, KITP, May 5 2020

Equilibrium predictions



Carnot efficiency

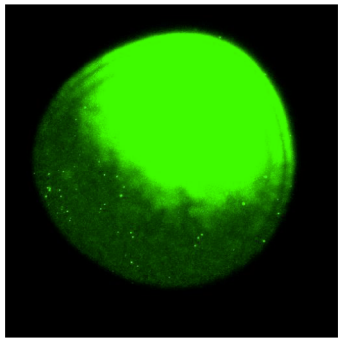
$$\eta \leq 1 - \frac{T_c}{T_h}$$

Universal energy constraint

Optimal engine design

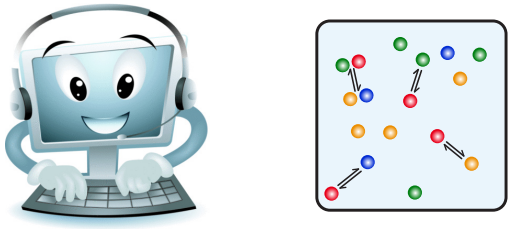
Nature is nonequilibrium

Patterns



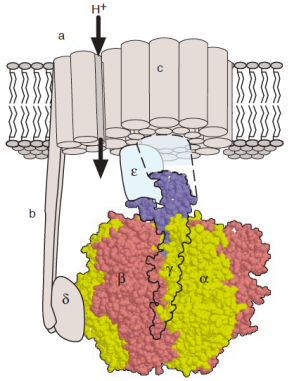
Fakhri Lab MIT

Information processing



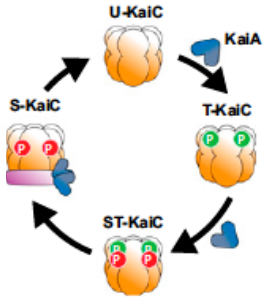
Beirut et. al. Nature (2012)

Molecular motors



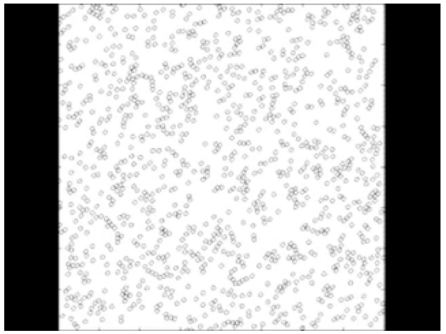
Wang/Oster Nature (1998)

Chemical clocks



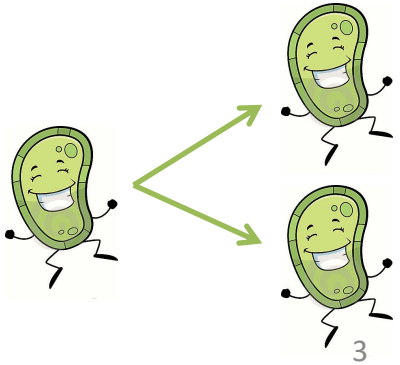
Rust PNAS (2012)

Active matter



Palacci et. al. Science (2013)

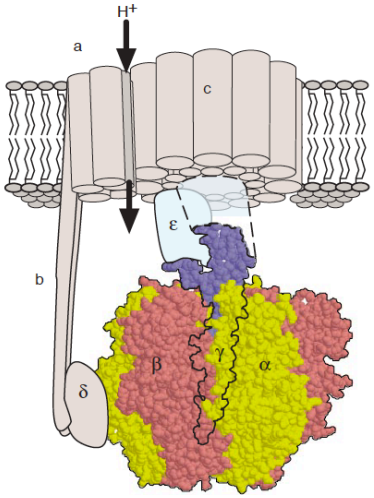
Replication



England JCP (2013)

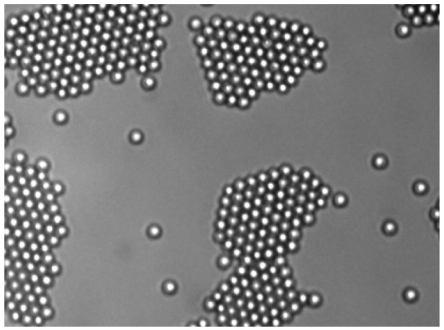
Nonequilibrium thermodynamics

Molecular motors



Wang/Oster Nature (1998)

Active matter



Palacci et. al. Science (2013)

Fundamental energetic limitations?

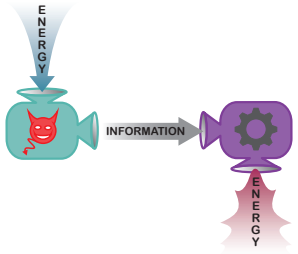
Rectify energy to do a useful task?

Material properties?

Research overview

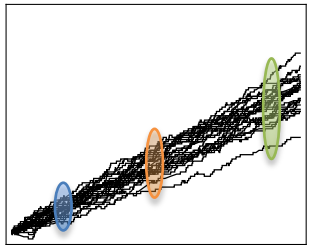
Horowitz Lab

Information



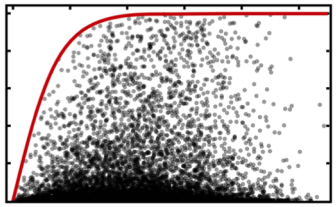
JMH/Esposito PRX 2014
JMH/Sagawa/Parrondo PRL 2013
JMH/Parrondo EPL 2011
JMH/Vaikuntanathan PRE 2010

Fluctuations



Gingrich/**JMH**/Perunov/ England PRL 2016
Gingrich/**JMH** PRL 2017
JMH/Gingrich PRE 2017
Marsland/Cui/**JMH** JRSI. 2020
JMH/Gingrich Nat. Phys. 2020

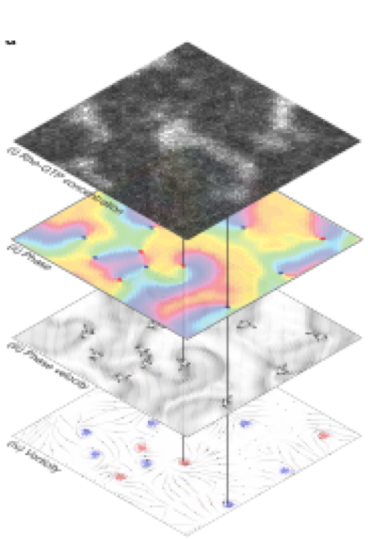
Response

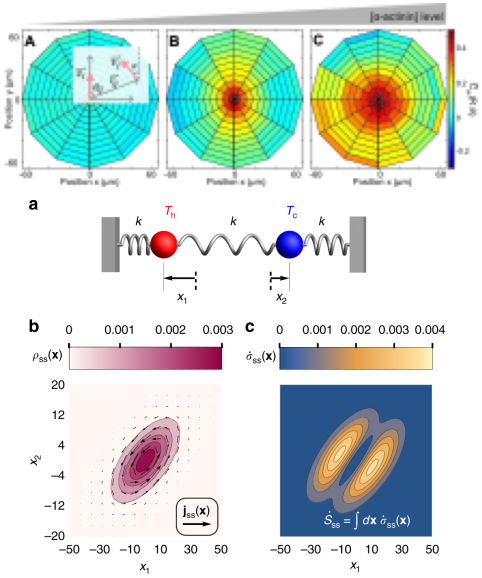


Owen/Gingrich/**JMH** PRX 2020

Fakhri Lab

Broken symmetries in living systems



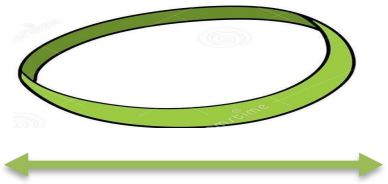


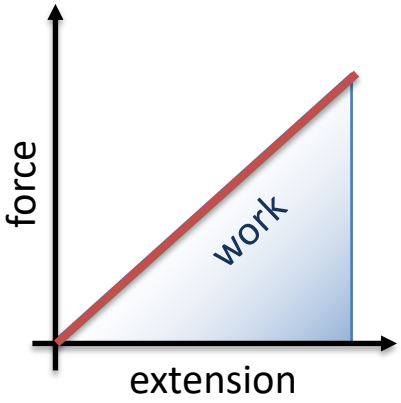
Fakhri et. al. Science 2014
Battle*, Broedersz*, Fakhri* et al. Science 2016
Gladrow, Fakhri et al. PRL 2016
Li, Horowitz, Gingrich, Fakhri. Nat Comm. 2019
Tan*, Warson*, Gingrich, Horowitz, Fakhri in revision

Tan et al. Sci Adv 2018
Tan, Liu, Miller, Tekant, Dunkel, Fakhri Nat Phys 2020
Wigbers*, Tan*, Brauns, Frey, Fakhri In revision

Thermodynamics structures fluctuations

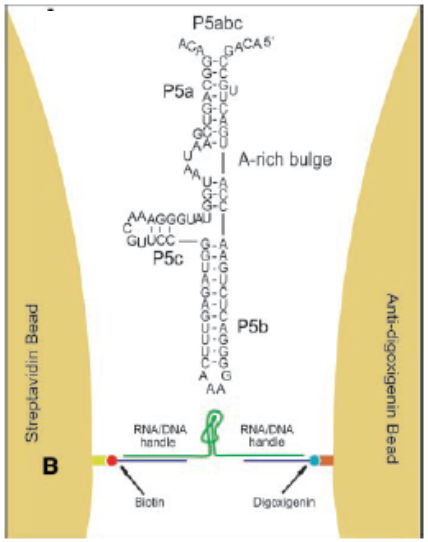
Rubber band

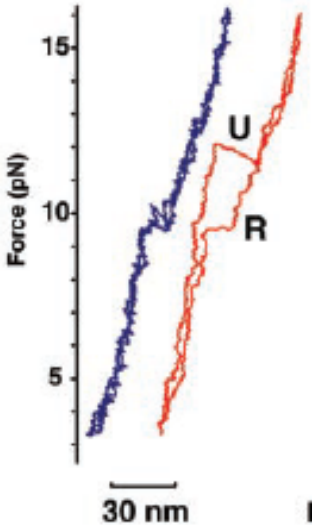




$$W \geq \Delta F$$

RNA Hairpin



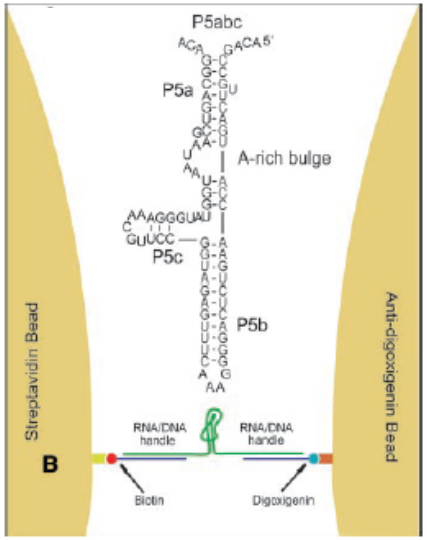


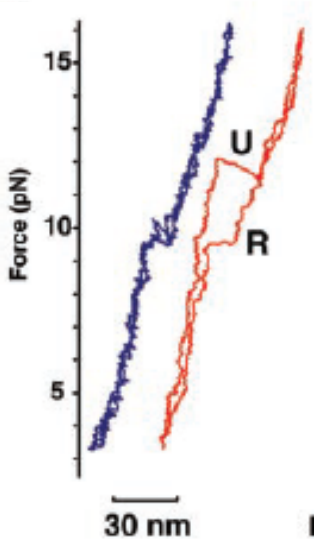
$$\langle W \rangle \geq \Delta F$$

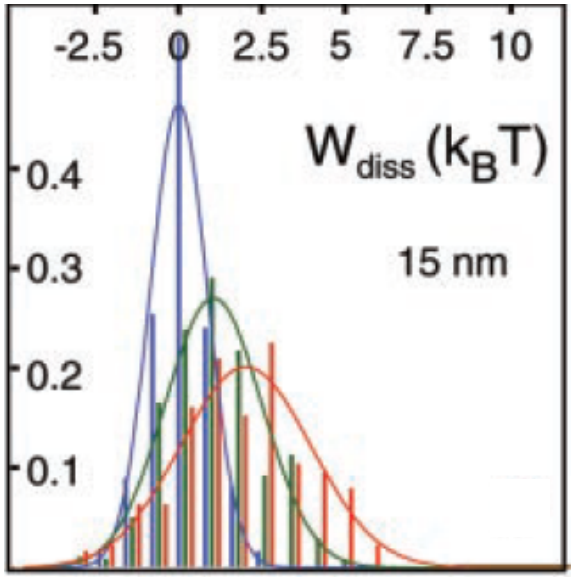
Liphardt et al. Science (2002)

Thermodynamics structures fluctuations: Jarzynski equality

RNA Hairpin







$$\left\langle e^{-\beta(W-\Delta F)} \right\rangle = 1$$

Liphardt et al. Science (2002)
Jarzynski, PRL (1997)

Stochastic thermodynamics

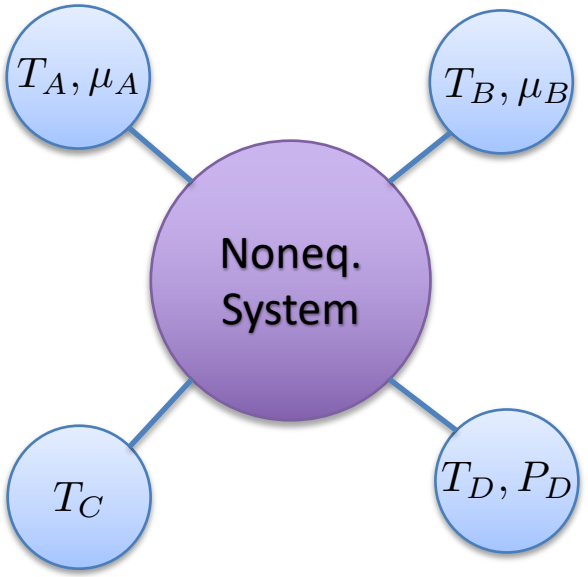
Dynamics linked to thermodynamics

The coupling of a system to many equilibrium thermodynamic reservoirs imposes specific constraints on the dynamics

Identifies fluctuating work,

heat, and entropy along

individual stochastic trajectories



Van den Broeck/Esposito Physica A (2002); Seifert, Rep. Prog. Phys. (2012)

Paradigm: driven colloid

Langevin equation

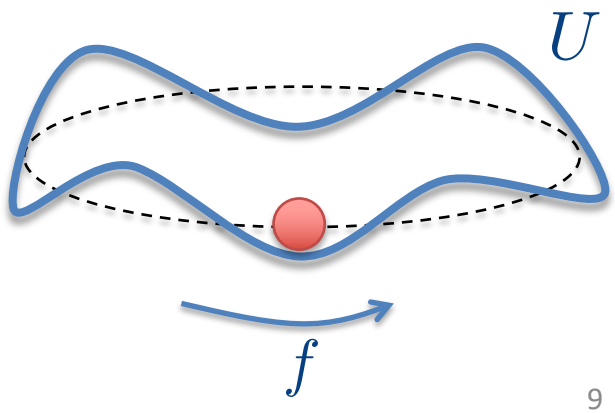
$$\gamma \dot{x}_t = -\partial_x U(x_t; \lambda_t) + f + \sqrt{2D}\xi_t$$

- $\gamma \dot{x}_t$: viscous damping
- $\partial_x U(x_t; \lambda_t)$: energy
- λ_t: external work parameter
- f: Non-conservative force
- $\sqrt{2D}\xi_t$: thermal noise

Dynamics-thermo link

fluctuation-dissipation theorem

$$D = \gamma k_{\mathrm{B}} T$$



1st Law: stochastic energetics

$$\underbrace{-\gamma\dot{x}_t + \sqrt{2\gamma k_{\mathrm{B}}T}\xi_t}_{\text{force due to reservoir}} \underbrace{- \partial_x U(x_t;\lambda_t) + f}_{\text{external forces}} = 0$$

Heat

work due to reservoir $\quad q_t = \int_0^t (\gamma\dot{x}_s - \sqrt{2\gamma k_{\mathrm{B}}}T\xi_s)dx_s$

Work $\quad w_t = \int_0^t \partial_\lambda U d\lambda_s + f dx_s$

Energy $\quad \Delta U_t = w_t - q_t$

Van den Broeck/Esposito Physica A (2002); Seifert, Rep. Prog. Phys. (2012)

2nd Law: stochastic entropy

Reservoir entropy change

$$\Delta s_t^{\mathrm{res}} = q_t/T$$

System entropy

$$s_t(x_t) = -k_{\mathrm{B}} \ln p_t(x_t)$$

Entropy production

$$\sigma_t = \Delta s_t + \Delta s_t^{\mathrm{res}}$$

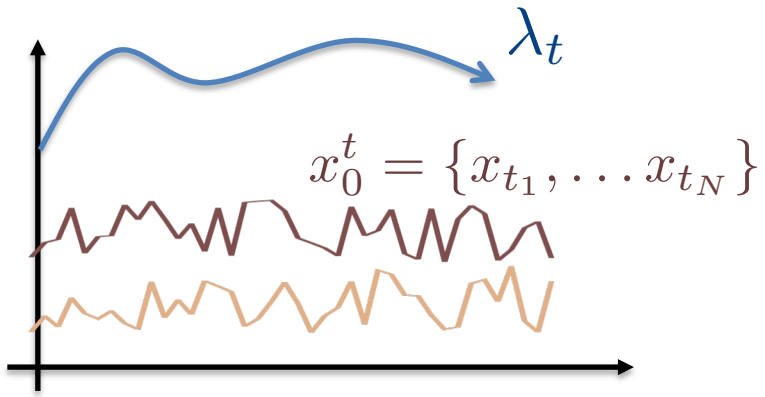
Van den Broeck/Esposito Physica A (2002); Seifert, Rep. Prog. Phys. (2012)

Irreversibility

Forward process

external parameter protocol

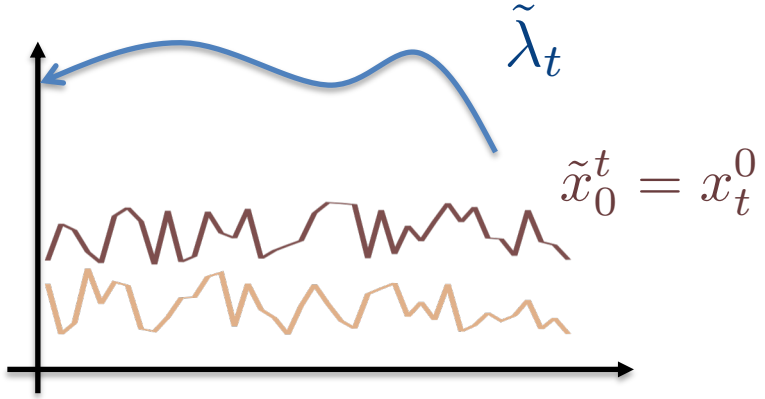
$\mathcal{P}[x_0^t]$



Reverse process

time-reversed protocol

$\tilde{\mathcal{P}}[\tilde{x}_0^t]$



Measuring entropy production with irreversibility

Detailed fluctuation theorem

$$\frac{\mathcal{P}[x_0^t]}{\tilde{\mathcal{P}}[\tilde{x}_0^t]} = e^{\sigma_t[x_0^t]}$$

Quantifying irreversibility

relative entropy –measure of distinguishability

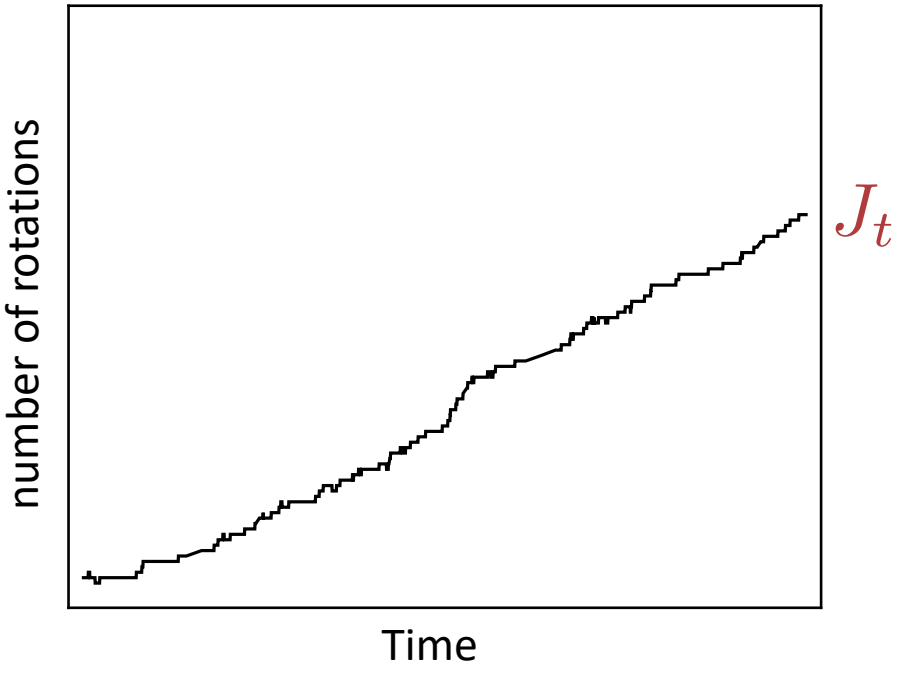
$$\Sigma_t = D(\mathcal{P}||\tilde{\mathcal{P}})$$

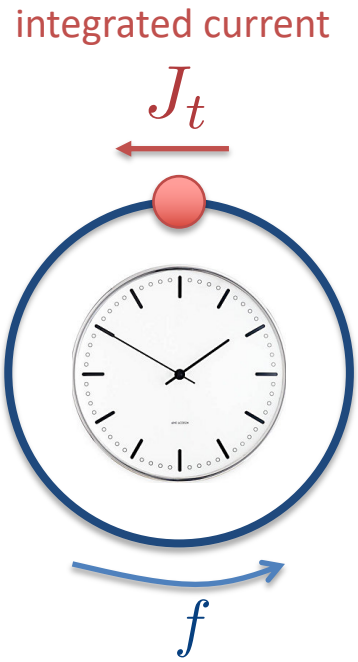
average entropy production $\langle \sigma_t \rangle$

$$\int \mathcal{D}[x_0^t]\ \mathcal{P}[x_0^t] \ln \frac{\mathcal{P}[x_0^t]}{\tilde{\mathcal{P}}[\tilde{x}_0^t]}$$

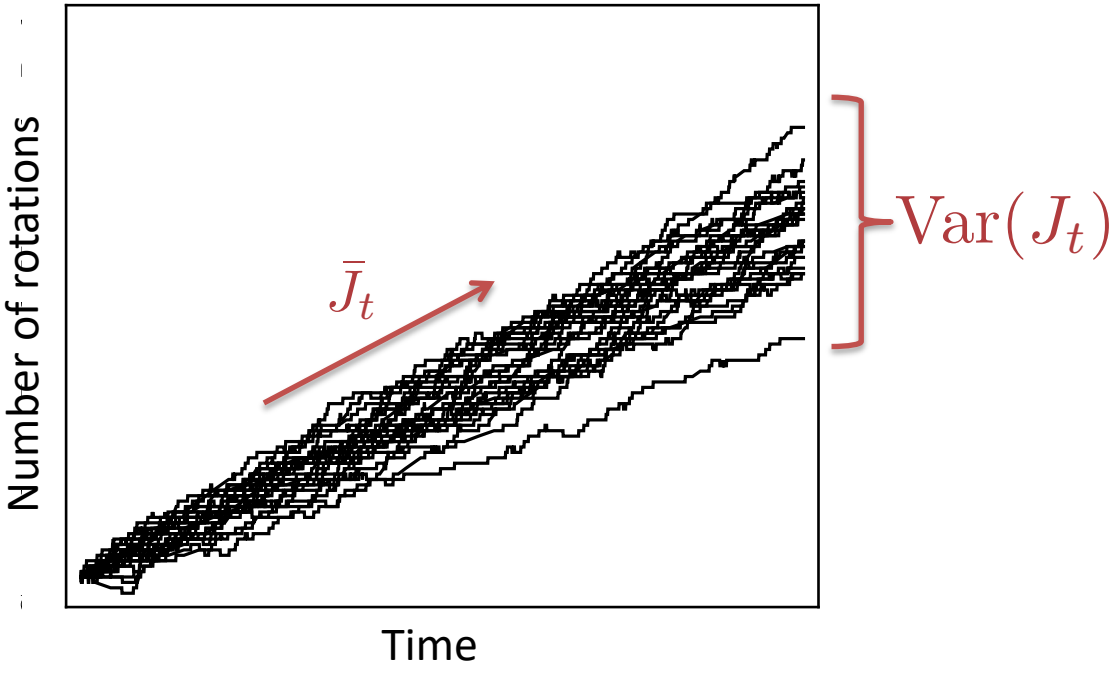
Parrondo et al. NJP (2009)

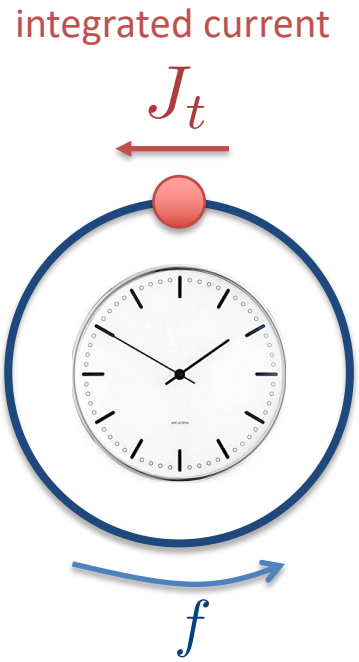
Steady-state currents fluctuate





Quantifying fluctuations





Precision costs energy

Thermodynamic uncertainty relation

relative uncertainty

$$\frac{\mathrm{Var}(J_t)}{\bar{J}_t^2} \geq \frac{2k_\mathrm{B}}{\Sigma_t}$$

energy dissipation

Currents: particle, energy, distance…

Tightest: near equilibrium, heat fluctuations

Gingrich/**JMH**/Perunov/England PRL (2016); **JMH**/Gingrich PRE (2017)
Barato/Seifert PRL (2015); Pietzonka/Ritort/Seifert PRE 96, 012101 (2017)

Applications

Power fluctuations in heat engines

Pietzonka/Seifert PRL (2018)

Efficiency of molecular motors

Pietzonka/Barato/Seifert J. Stat. Mech. (2016)

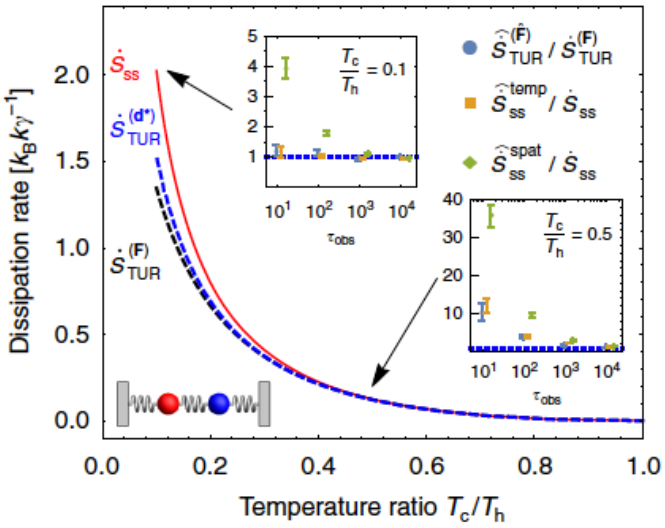
Estimate dissipation from current fluctuations

Li/**JMH**/Gingrich/**Fakhri** Nat. Comm. (2020)

Manikandan/Gupta/Krishnamurthy PRL (2020)

Otsubo/Ito/Dechant/Sagawa arxiv (2020)

Vu/Vo/Hasegawa PRE, 101, 042138 (2020)



So far…

Stochastic thermodynamics offers a theoretical framework for consistent thermodynamic accounting along individual stochastic trajectories

…Up next

Application of stochastic thermodynamic tools to complex nonequilibrium matter opens new insights into the mechanisms of dissipation

Acknowledgements

Faculty

Todd Gingrich (Northwestern)

Jeremy England (GSK)

Nikta Fakhri (MIT)

Postdocs

Robert Marsland (BU)

Karel Proesmans (Simon Fraser)

Graduate students

Nikolai Perunov (MIT)

Jeremy Owen (MIT)

Wei Cui (BU)

Review articles

Stochastic thermodynamics

- Van den Broeck/Esposito, Physica A, 418, 6-16 (2015)
- Seifert, Rep. Prog. Phys. 75, 126001 (2012)
- Jarzynski Ann. Rev. Cond. Matt. Phys. 2, 329-351 (2011)

Information thermodynamics

- Parrondo/**JMH**/Sagawa Nat. Phys. 11, 131-139 (2015)

Thermodynamic uncertainty relations

- **JMH**/Gingrich Nat. Phys. 16, 15-20 (2020)

Experiments

- Ciliberto PRX 7, 021051 (2017)