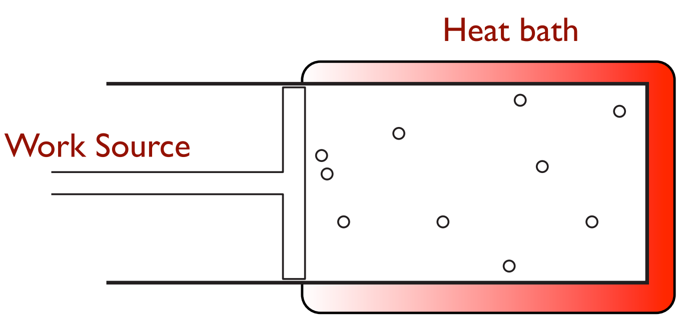
On the thermodynamics of strongly coupled systems

Gavin Crooks & Susanna Still

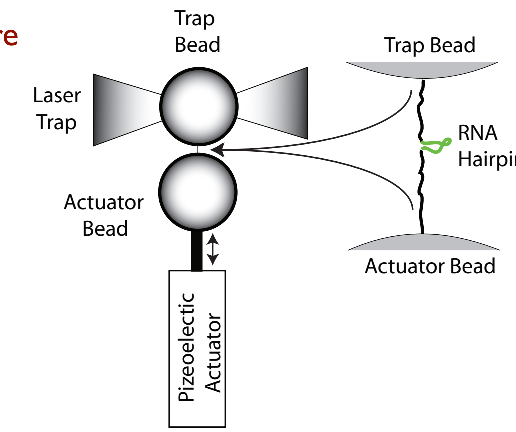
Telluride 2016



forward trajectory — forward control — inverse temperature — Heat

$$\ln \frac{p(\overrightarrow{x}|\overrightarrow{u}, x_0)}{p(\overleftarrow{x}|\overleftarrow{u}, \tilde{x}_\tau)} = -\beta Q$$

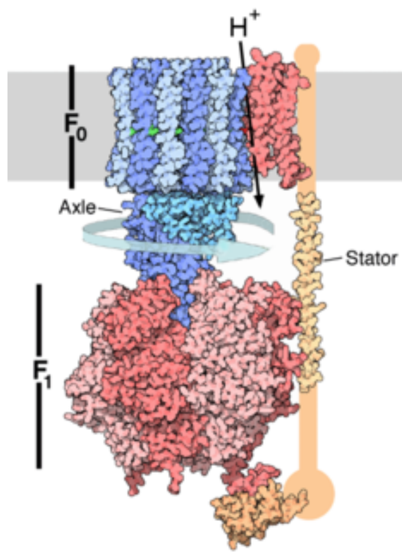
reversed trajectory — reversed control

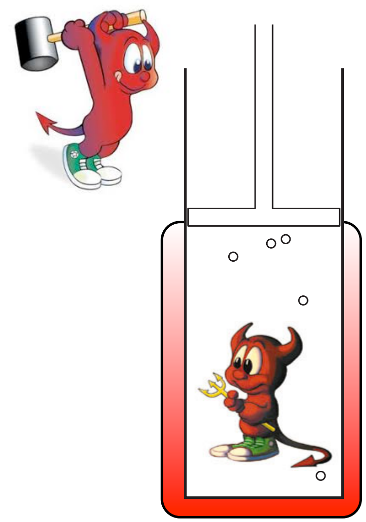


Slides: http://threeplusone.com/telluride2016

On the thermodynamics of strongly coupled systems

Gavin Crooks & Susanna Still
Telluride 2016

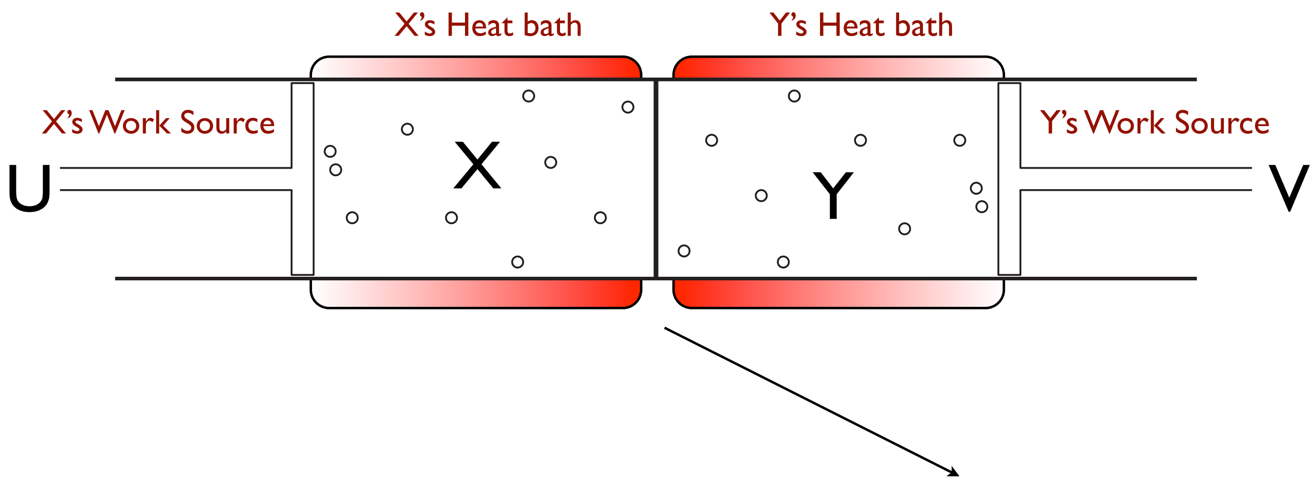




Open problem: Most of reality doesn't consist of weakly coupled systems.

Slides: http://threeplusone.com/telluride2016

Detailed Fluctuation Theorem: Coupled systems



$$E_{XY}(x, y; u, v) = E_X(x; u) + E_Y(y; v) + E^{\text{int}}_{X:Y}(x, y)$$

joint entropy production

$$\Sigma_{XY} = \ln \frac{p(\vec{x}, \vec{y}; \vec{u}, \vec{v})}{p(\overleftarrow{x}, \overleftarrow{y}; \overleftarrow{u}, \overleftarrow{v})}$$

$$\Sigma_{XY} = \Sigma^{\text{sys}}_{XY} + \Sigma^{\text{env}}_{XY}$$
$$= \Delta s_{XY} - \beta Q_X - \beta Q_Y$$

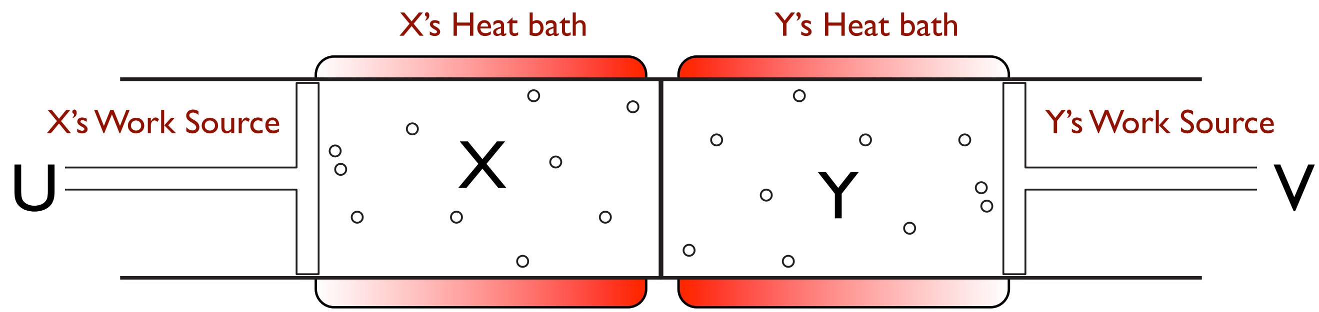
pointwise entropy change

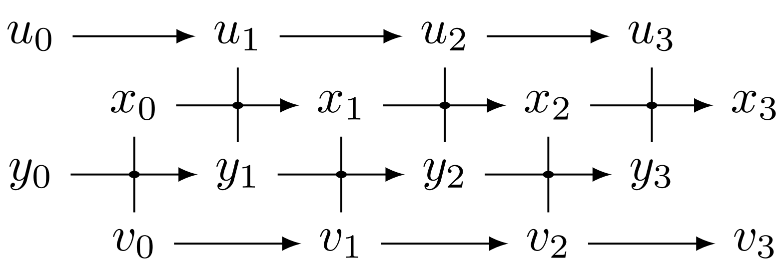
Heat

marginal entropy production

$$\Sigma_X = \ln \frac{p(\vec{x})}{p(\overleftarrow{x})} \quad \textbf{=?}$$

Dynamics: Conditionally Markov





$$
\begin{aligned}
p(\vec{x}, \vec{y} \mid x_0, y_0) \\
&= p(y_1 \mid y_0, x_0)\, p(x_1 \mid x_0, y_1)\, p(y_2 \mid y_1, x_1)\, p(x_2 \mid x_1, y_2) \\
&\quad \ldots p(y_\tau \mid y_{\tau-1}, x_{\tau-1})\, p(x_\tau \mid x_{\tau-1}, y_\tau) \\
&= \prod_{t=0}^{\tau-1} p(y_{t+1} \mid y_t, x_t) \prod_{t=0}^{\tau-1} p(x_{t+1} \mid x_t, y_{t+1}) \\
&= q(\vec{y}; \vec{x}, y_0)\, q(\vec{x}; \vec{y}, x_0)
\end{aligned}
$$

See: "do calculus"
in "Causality" by Judea Pearl (2000)

No Feedback
These Are NOT the conditional distributions!!!

Marginal fluctuation theorem

$$\Sigma_X = \ln \frac{p(\vec{x})}{p(\overleftarrow{x})}$$

$$= \ln \frac{p(\vec{x}, \vec{y})}{p(\overleftarrow{x}, \overleftarrow{y})} \frac{p(\overleftarrow{y}|\overleftarrow{x})}{p(\vec{y}|\vec{x})}$$

$$= \ln \frac{p(\vec{x}, \vec{y}|x_0, y_0)}{p(\overleftarrow{x}, \overleftarrow{y}|\tilde{x}_\tau, \tilde{y}_\tau)} \frac{p(x_0, y_0)}{p(\tilde{x}_\tau, \tilde{y}_\tau)} \frac{p(\overleftarrow{y}|\overleftarrow{x})}{p(\vec{y}|\vec{x})}$$

$$= \ln \frac{q(\vec{y}; \vec{x}, y_0)\, q(\vec{x}; \vec{y}, x_0)}{q(\overleftarrow{y}; \overleftarrow{x}, \tilde{y}_\tau)\, q(\overleftarrow{x}; \overleftarrow{y}, \tilde{x}_\tau)} \frac{p(y_0|x_0)}{p(\tilde{y}_\tau|\tilde{x}_\tau)} \frac{p(x_0)}{p(\tilde{x}_\tau)} \frac{p(\overleftarrow{y}|\overleftarrow{x})}{p(\vec{y}|\vec{x})}$$

$$= \ln \frac{p(x_0)}{p(\tilde{x}_\tau)} + \ln \frac{q(\vec{x}; \vec{y}, x_0)}{q(\overleftarrow{x}; \overleftarrow{y}, \tilde{x}_\tau)} - \ln \frac{p(\vec{y}|\vec{x})}{p(\overleftarrow{y}|\overleftarrow{x})} + \ln \frac{q(\vec{y}; \vec{x})}{q(\overleftarrow{y}; \overleftarrow{x})}$$

$$= +\Delta s_X - \beta Q_X - \Sigma_X^{trn}$$

$$p(\vec{x}, \vec{y} \mid x_0, y_0) = q(\vec{y}; \vec{x}, y_0)\, q(\vec{x}; \vec{y}, x_0)$$

$$\ln \frac{q(\vec{x}|\vec{y}, x_0)}{q(\overleftarrow{x}|\overleftarrow{y}, \tilde{x}_\tau)} = -\beta Q_X$$

Transferred dissipation $\Sigma_X^{trn} = \ln \frac{p(\vec{y}|\vec{x})}{p(\overleftarrow{y}|\overleftarrow{x})} - \ln \frac{q(\vec{y}; \vec{x})}{q(\overleftarrow{y}; \overleftarrow{x})}$

Local Second Laws

$$\Sigma_X = \Delta s_X - \beta Q_X - \Sigma_X^{trn}$$

$$\langle \Sigma_X \rangle = \sum_{\vec{x}} p(\vec{x}) \ln \frac{p(\vec{x})}{p(\overleftarrow{x})} \geqslant 0$$

$$\Delta S_X - \beta \langle Q_X \rangle \geqslant \langle \Sigma_X^{trn} \rangle$$

joint 2nd law *marginal and conditional 2nd laws*

$$\langle \Sigma_{\vec{X},\vec{Y}} \rangle \geq \left\{ \langle \Sigma_{\vec{X}} \rangle, \langle \Sigma_{\vec{Y}} \rangle, \langle \Sigma_{\vec{X}|\vec{Y}} \rangle, \langle \Sigma_{\vec{Y}|\vec{X}} \rangle \right\} \geq 0$$

Transient Protocols

Excess dissipation $\Sigma_X^{ex} = -\beta\Delta F_X + \beta W_X + L_X^{trn}$

Transferred Labor $L_X^{trn} = -\beta\Delta F_{Y|X} - \ln\langle e^{-\beta W_Y}\rangle$ ← *Feedback correction terms can be measured!*

$$\sum_{\overleftarrow{y}} p(\overleftarrow{x},\overleftarrow{y}) = \sum_{\overrightarrow{y}} p(\overrightarrow{x},\overrightarrow{y}) e^{-\Sigma_{XY}}$$

$$p(\overleftarrow{x}) = p(\overrightarrow{x}) \sum_{\overrightarrow{y}} p(\overrightarrow{y}|\overrightarrow{x}) e^{-\Sigma_{XY}}$$

$$\ln \frac{p(\overrightarrow{x})}{p(\overleftarrow{x})} = +\Delta s_X - \beta\Delta E_X + \beta W_X - \ln \sum_{\overrightarrow{y}} p(\overrightarrow{y}|\overrightarrow{x}) e^{-\Delta s_Y + \Delta E_Y - \beta W_Y + \Delta i_{X:Y} + \Delta E^{int}_{X:Y}}$$

Local 1st Law

$$\beta E_Y^{trn} = L_Y^{trn} + \Sigma_Y^{trn}$$

Transferred Energy — *Transferred Labor* — *Transferred Dissipation*

Open Problem: Can we use these measures to sensible partition a system into semi-independent parts?

Idealizations

Local 1st Law

$$\beta E_Y^{trn} = L_Y^{trn} + \Sigma_Y^{trn}$$

Transferred Energy *Transferred Labor* *Transferred Dissipation*

Other system relaxes fast — Ideal heat bath

Other system does not react — Ideal work source

No energy flow — Demons (computational resources)

& no feedback in reverse time — Feedback reversible demons

& no feedback to the system — Ideal measurement (Bayesian FT)

See also: Deffner and Jarzynski (2013)

Slides: http://threeplusone.com/telluride2016

Feedback reversible fluctuation theorem (1)

$$\Sigma_X^{\mathrm{trn}} = \ln \frac{p(\vec{y}|\vec{x})}{q(\vec{y};\vec{x})} - \ln \frac{p(\overleftarrow{y}|\overleftarrow{x})}{q(\overleftarrow{y};\overleftarrow{x})}$$

No feedback in time-reverse dynamics

$$T_{Y\to X} = \ln \frac{p(\vec{y}|\vec{x})}{q(\vec{y};\vec{x})} = \ln \frac{p(\vec{y},\vec{x}|x_0,y_0)}{q(\vec{y};\vec{x},y_0)\,p(\vec{x}|x_0)}$$

$$= \ln \frac{q(\vec{x};\vec{y},x_0)}{p(\vec{x}|x_0)}$$

$$= \ln \prod_{t=0}^{\tau-1} p(x_{t+1} \mid x_t, y_{t+1}) - \ln \prod_{t=0}^{\tau-1} p(x_{t+1} \mid x_{0:t})$$

$$= \sum_{t=0}^{\tau-1} \ln \frac{p(x_{t+1} \mid x_{0:t}, y_{0:t+1})}{p(x_{t+1} \mid x_{0:t})}$$

$$= \sum_{t=0}^{\tau-1} i(x_{t+1} : y_{0:t+1} \mid x_{0:t})$$

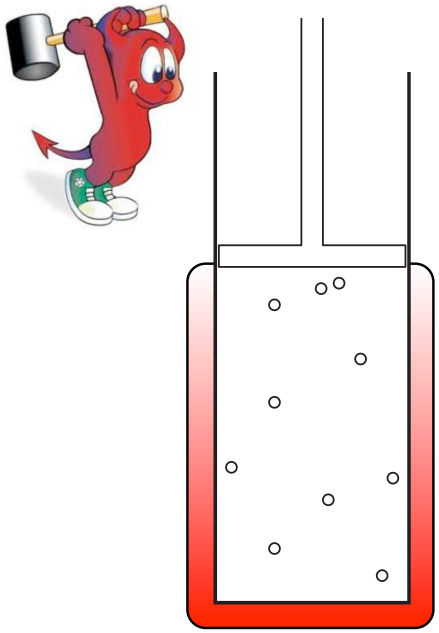
Transfer Entropy

Feedback reversible fluctuation theorem (2)

$$\langle \Sigma_X^{\mathrm{trn}} \rangle = \langle T_{X\to Y} \rangle \geqslant 0,$$

No feedback in time-reverse dynamics

$$\Delta S_X - \beta \langle Q_X \rangle \geqslant \langle \Sigma_X^{\mathrm{trn}} \rangle$$
$$\Delta S_X - \beta \langle Q_X \rangle \geqslant \langle T_{X\to Y} \rangle \geqslant 0$$
$$\Delta S_X - \beta \langle Q_X \rangle \geqslant \Delta I_{X:Y} - \langle T_{Y\to X} \rangle$$



Sagawa & Ueda (2010)
Horowitz & Vaikuntanathan (2010)