

Thermodynamically optimal processes with memory



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Non-equilibrium thermodynamics: from chemical reactions to machine learning Higgs Centre, University of Edinburgh





[M.C. Engel, J.A. Smith, M.P. Brenner, PRX (2023)] [S. Blaber, D. A Sivak, J. Phys. Commun. 7 033001 (2023)]

Most thermodynamically efficient way to bring system from A to B in finite time?



[L. K. Davis, K. Proesmans, and É. Fodor, PRX (2024)]





Microscale processes as "<u>machines</u>"



Biology: Has evolution lead to energy-optimisation?

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External work input (ATP, external forcing,...) Motion against friction: heat production Thermodynamic processes as "machines" **Efficiency?**

"Swallow the surgeon" – R. Feynman

Engineering: How to build most efficient robots?







Microscale processes as "machines"



Challenges at microscale:

- High friction
- (Non-)thermal noise

*slow, hidden D.O.F. that participate in dynamics but are not directly controllable or measurable (non-Markovianity)

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 Memory*, e.g., from internal D.O.F. or from viscoelastic environment (cytoskeleton, blood...)







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Loos, Monter, Ginot, Bechinger, Physical Review X 14, 021032 (2024)

Garcia-Millan, Schuettler, Cates, Loos, ArXiv:2407.18542 (2024)

Schuettler, Garcia-Millan, Cates, Loos, ArXiv:2501.18613 (2025)

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Background: Stochastic thermodynamics and optimal control

The optimal dragging problem

Impact of memory and the role of symmetry

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Outline







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Paradigmatic model: Markovian Langevin equation



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white Gaussian noise : $\langle \xi \rangle = 0$, $\langle \xi(t)\xi(t') \rangle = 2k_BT \,\delta(t-t')$

 \rightarrow "Markovian" = no memory, if timescale separation between "system" and "bath"







<u>Stochastic work and heat:</u>



Stochastic entropy production:

 $S_{\rm sys}(x) \propto -\ln\rho(x)$

Seifert, PRL 95, 040602 (2005), Sekimoto, Stochastic Energetics, Springer 2010

= ln



 \Rightarrow 1st law : $\mathrm{d}V = \delta w + \delta q \checkmark$

 $\Rightarrow \delta q = [-\gamma \dot{X}(t) + \xi(t)] \circ dX$

 $\int_0^1 \delta q$ $P[\{\mathbf{X}(t')\}_{0}^{t}]$ \Rightarrow 2nd law: $\Delta S_{\rm sys}$ $\hat{P}[\{\hat{\mathbf{X}}(t')\}_{0}^{t}]$ $\langle \Sigma \rangle \geq 0$ 🗸



Non-Markovian case: Generalised Langevin equation

(Non-Markovian) Generalized Langevin equation: $m\ddot{X}(t) + \int_{-\infty}^{t} \Gamma(t - t')\dot{X}(t')dt' = -\nabla_X V(X)$

retarded friction

Fluctuation-Dissipation Relation: $\Gamma(|t - t'|) \propto \langle \nu(t)\nu(t') \rangle$ (Equilibrium)

Dimensionality given by spectrum of Γ , in general ∞ -dimensional process

- [Esposito. Phys. Rev. E (2012)]
- Acausality of backward process: [Rosinberg, Tarjus, & Munakata, PRE (2017), Loos & Klapp, Sci. Rep. (2019), Loos & Klapp, NJP (2021), ...]

$$(X,\lambda) + \underline{\eta(t)}$$

coloured noise



- <u>Hidden D.O.F.</u>: "No idea" how much entropy we are missing ($\Sigma^{\text{coarse-gr.}} \leq \Sigma^{\text{full}}$) $\Sigma = \ln \frac{P[\{\mathbf{X}(t')\}_{0}^{t}]}{\hat{P}[\{\hat{\mathbf{X}}(t')\}_{0}^{t}]} = \frac{\int_{0}^{t} \delta q}{T} + \Delta S_{\text{sys}} + \Delta I$ "information-flow between presence and past"





Thermodynamic process with "additional d.o.f."

External WORK

Viscoelastic fluid ELASTIC ENERGY

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Thermodynamically optimal control



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Most thermodynamically efficient way to bring system from A to B in finite time?

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Thermodynamically optimal control — General results so far

• Optimal control theory, variational calculus (Euler-Langrange eq.) + Stochastic calculus

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stiffness $\lambda(t)$

trap

Exact results (Gaussian systems)

Discontinuities of protocol $\lambda(t)$ at beginning and end = "bang-bang solutions"

[Schmiedl & Seifert, PRL 98, 10830 (2007)]

• Jumps generic for "fast-protocol" ($t_f \rightarrow 0$) solutions [S. Blader, M.D. Louwerse, D.A. Sivak, PRE (2021)]

• For nonlinear systems: Approximative schemes

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Side note: Thermodynamically optimal control of nonlinear systems

• For nonlinear systems: Geometric approach based on response theory

[Crooks, PRL (2007)] [Zhong, DeWeese, PRE (2022)] [Sivak, Crooks, PRL (2012)] [Van Vu and Saito, PRX (2023)]



*[S. Blader, M.D. Louwerse, D. A. Sivak, PRE (2021)]

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Optimal control problem:



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The optimal dragging problem

Protocol to move λ from $\lambda(0) = \lambda_0$ to $\lambda(t_f) = \lambda_f$ in time t_f that minimises average work $\langle W[x,\lambda] \rangle$?

...Simple enough to study analytically!



Work spend along dragging: ullet



- λ : Trap center
- X: particle position





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$$W[X(t), \lambda(t)] = \int_0^{\lambda_{\rm f}} \frac{\partial V}{\partial \lambda} \circ d\lambda = \kappa \int_0^{\lambda_{\rm f}} \dot{\lambda}(\lambda - X) \circ dt$$



Samuel Monter Universität Felix Ginot Konstanz **Clemens Bechinger**



[Schmiedl & Seifert, PRL 98, 10830 (2007)]



Work spend along dragging.



• Particle in viscous fluid:





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Minimum work dragging problem: viscous case Steady state Steady state

$$\bigvee V = \frac{\kappa}{2} [X - \lambda(t)]^2$$

$$W[X(t),\lambda(t)] = \int_0^{\lambda_{\rm f}} \frac{\partial V}{\partial \lambda} \circ d\lambda = \kappa \int_0^{\lambda_{\rm f}} \dot{\lambda}(\lambda - X)$$

$$\tau_0 \dot{X} = -\left[X - \lambda(t)\right] + \xi \quad \tau_0 = \gamma_0 / \kappa$$
$$\langle \xi(t)\xi(t') \rangle \propto \delta(t - t')$$

Euler-Langrange Eq.

Optimal protocol:

$$\lambda^*(t) = \begin{cases} 0, & t = 0\\ \Delta \lambda^*(1 + t/\tau_0), & 0 < t < t_{\rm f}, \\ \lambda_{\rm f}, & t = t_{\rm f} \end{cases}$$
$$\Delta \lambda^* = \tau_0 / (t_{\rm f} + 2\tau_0) \lambda_{\rm f}$$

[Schmiedl & Seifert, PRL 98, 10830 (2007)]



Work spen \bullet



Langevin equ





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Optimal protocol:

$$\lambda^*(t) = \begin{cases} 0, & t = 0\\ \Delta \lambda^*(1 + t/\tau_0), & 0 < t < t_{\rm f}, \\ \lambda_{\rm f}, & t = t_{\rm f} \end{cases}$$
$$\Delta \lambda^* = \tau_0 / (t_{\rm f} + 2\tau_0) \lambda_{\rm f}$$

[Schmiedl & Seifert, PRL 98, 10830 (2007)]







Minimum work dragging problem: viscous case



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 $r = 2.7 \,\mu{\rm m}$



Minimum work dragging problem, non-Markovian case

1_f



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Wormlike micelles/ polymer solution

8mM mixture of CPyCI and NaSal



 $t_{\rm f} = 10 \,\text{s}, \ r = 2.7 \,\mu\text{m}$ $\lambda_{\rm f} = 3 \,\mu\text{m} \qquad \tau_{\rm b} \approx 17 \,s$





Minimum work dragging problem, non-Markovian case



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(non-Markovian) Generalized Langevin equation:

 $\tau_0 \dot{X}(t) + \int_{-\infty}^{t} \Gamma(t - t') \dot{X}(t') dt' = -V' + \xi(t) + \underbrace{\eta(t)}_{-\infty}$

coloured noise

retarded friction

 $\langle \eta(t) \rangle = 0$

"Maxwell model": $\Gamma(t-t') \propto \langle \eta(t)\eta(t') \rangle \propto \sum e^{-|t-t'|/\tau_{\mathrm{b,i}}}$ Memory time: τ_{b}









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$$\left[2\tau_p \mathcal{C}_1 + \tau_b \mathcal{C}_2 + \tau_b (2\mathcal{C}_1 - \mathcal{C}_2) \cosh \frac{\sqrt{\tau_b + \tau_p}}{\tau_b \sqrt{\tau_p}} t - \tau_b \frac{\sqrt{\tau_b + \tau_p}}{\sqrt{\tau_p}} \sinh \frac{\sqrt{\tau_b + \tau_p}}{\tau_b \sqrt{\tau_p}} t\right]$$

$$rac{1}{k}\left[2 au_p(au_b+ au_p+kt)\mathcal{C}_1+ au_b(au_b+ au_p+ au_bk+kt)\mathcal{C}_2
ight.$$

$$(z_b + \tau_b k) \mathcal{C}_2 \cosh \frac{\sqrt{\tau_b + \tau_p}}{\tau_b \sqrt{\tau_p}} t + \frac{\tau_b \sqrt{\tau_p} (\tau_b + \tau_p + \tau_b k) (2\mathcal{C}_1 - \mathcal{C}_2)}{\sqrt{\tau_b + \tau_p}} \sinh \frac{\sqrt{\tau_b + \tau_p}}{\tau_b \sqrt{\tau_p}} t$$



Minimum work dragging problem, non-Markovian case

- Viscous Markovian case (black line)
- Viscoelastic non-Markovian case (red line)



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\rightarrow Still jumps at beginning and end **line)** \rightarrow No constant-power "NESS regime"

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$$f = \{\langle X \rangle, \lambda\}$$
Time-reversal symmetry

$$f(t) = f(t_{\rm f}) - f(t_{\rm f} - t)$$

$$\dot{f}(t) = -\dot{f}(t_{\rm f})$$



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try — criterion for optimality

Dptimal solutions: $\langle X \rangle$ and λ are **time-reversal symmetric** $\rightarrow Why??$



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Time-reversal symmetry — criterion for optimality

Time-reversal symmetry
$$f(t) = f(t_f) - f(t_f - t)$$
 $f = \{\langle X \rangle, \lambda\}$

Proof of Symmetry: General Generalized Langevin E (GGLE)

$$m\ddot{X} + \int_{-\infty}^{t} \Gamma(t - t')\dot{X}(t')dt' = -\kappa[X - t]$$

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 $\lambda(t) + \eta(t)$

Proof using <u>linearity</u> of GGLE, <u>causality</u>, and <u>time-translation</u> invariance of response function and memory kernel Γ ...







Proof of symmetry property

<u>General Generalized Langevin Equation (GGLE)</u> $m\ddot{X} + \int_{-\infty}^{t} \Gamma(t - t')\dot{X}(t')dt' = -\kappa[X - \lambda(t)] + \eta(t)$

Counterexample I: Linear protocol





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Counterexample II: Single jump protocol





Proof of symmetry property

Key Idea: rewrite mean work as functional of λ (or \dot{x}) only!

$$\begin{split} & \underset{\text{for equivalence}}{\text{In } \ddot{X} + \int_{-\infty}^{t} \Gamma(t - t') \dot{X}(t') dt' = -\kappa [X - \lambda(t)]} \\ & \left\langle W[X(t), \lambda(t)] \right\rangle = \kappa \int_{0}^{t_{\text{f}}} dt \, \dot{\lambda}(t) \left[\lambda(t) - x \right] \\ & \hat{x}(s) = \hat{\Phi}(s) s \hat{\lambda}(s), \\ & \hat{\Phi}(s) \coloneqq \frac{\kappa}{ms^{3} + \hat{\Gamma}(s)s^{2} + \kappa s} \end{split} \end{split}$$

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Key Idea: rewrite mean work as functional of λ (or \dot{x}) only!

$$\left\langle W \right\rangle [\lambda] = rac{\kappa \lambda_{\mathrm{f}}^2}{2} + \kappa \int_0^{t_{\mathrm{f}}} \int_0^t \Phi(t - t') \dot{\lambda}(t) \dot{\lambda}$$

<u>Quadratic</u> functional of λ only:

 \rightarrow invariant under time reversal: $\lambda(t) \rightarrow - \lambda(t_{\rm f} - t)$ $\rightarrow \tilde{\lambda}(t) = -\lambda(t_{\rm f} - t) + \lambda(t_{\rm f})$ and $\lambda(t)$ give same work \rightarrow quadratic functional: can only have unique optimum

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Same argument for $\dot{x} = \langle \dot{X} \rangle$!

$$\begin{split} \langle W \rangle [x] &= \int_0^{t_{\rm f}} \int_0^t \Gamma(t-t') \dot{x}(t) \dot{x}(t') dt' dt + \\ &+ \kappa [x(t_{\rm f}) - \lambda_{\rm f}]^2 / 2 + \mathcal{C}, \end{split}$$

<u>Quadratic</u> functional of $\hat{\lambda}$ only:

 \rightarrow invariant under time reversal: $\lambda(t) \rightarrow -\lambda(t_{\rm f}-t)$ $\rightarrow \tilde{\lambda}(t) = -\lambda(t_{\rm f} - t) + \lambda(t_{\rm f})$ and $\lambda(t)$ give same work \rightarrow quadratic functional: can only have unique optimum

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Proof of symmetry property

$$m\ddot{X} + \int_{-\infty}^{t} \Gamma(t - t')\dot{X}(t')dt' = -\kappa[X - \lambda(t)]$$

$$\langle W \rangle [x] = \int_0^{t_{\rm f}} \int_0^t \Gamma(t - t') \dot{x}(t) \dot{x}(t') dt' dt + m[\dot{x}^2(t_{\rm f})]/2$$
$$+ \kappa [x(t_{\rm f}) - \lambda_{\rm f}]^2/2 + \mathcal{C},$$

Optimality! $\delta x(0) = \delta x(t_{\rm f}) = 0,$ $\delta \langle W \rangle \left[x(t), \delta x(t) \right] = 0$

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1) "⇔" : Symmetry <u>exclusive</u> to optimal case \rightarrow Criterion to find optimal processes

Asymmetry as alternative cost functional Value at minimum a priori known!



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2) Symmetry for GGLEs : <u>universal*</u> property \rightarrow also for e.g. granular or glassy media, and active baths





Outlook (I): Optimal dragging of active particles



Generalized Langevin equation: $\tau_0 \dot{X}(t) = -\left[X - \lambda(t)\right] + \xi(t) + \eta(t)$

[D Gupta, SHL Klapp, DA Sivak, PRE 108 (2), 024117 (2023)] [L. K. Davis, K. Proesmans, and É. Fodor, PRX (2024)] [Garcia-Millan*, Schuettler*, Cates, Loos, ArXiv:2407.18542 (2024)] [Schuettler, Garcia-Millan, Cates, Loos, ArXiv:2501.18613 (2025)]

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White noise (viscous medium) $\langle \xi(t)\xi(t')\rangle \propto \delta(t-t')$

Coloured noise (activity) $\langle \eta(t)\eta(t')\rangle \propto e^{-|t-t'|/\tau_{\rm b}}$

Active Ornstein-Uhlenbeck particle (AOUP)/ Run-and-Tumble particle (RTP)







Optimal closed-loop (feedback) control

Measurement of system state \rightarrow Allows to extract work (on average)

X measurement allows instantaneous work extraction from potential energy



[D. Abreu and U. Seifert, EPL (2011).]

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Optimal closed-loop (feedback) control

Allow one measurement at the beginning: Is the particle heading left or right?



Framework of information thermodynamics (Maxwell demon): Information-to-work conversion

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[D. Abreu and U. Seifert, EPL (2011).]







Outlook (II): Optimal dragging through critical medium



Steady state driving (quasi static regime):

[Venturelli*, Walter*, Loos*, Roldan, Gambassi, EPL 146, 27001 (2024)]

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 $\mathcal{H}[\phi, \mathbf{Y}, t] = \mathcal{H}_{\phi}[\phi] + \mathcal{H}^{\text{int}}[\phi, \mathbf{Y}] + \mathcal{U}(\mathbf{Y}, t)$

$$\begin{split} \gamma_{y} \dot{\mathbf{Y}} &= -\nabla_{\mathbf{Y}} \mathcal{H} + \mathbf{F}_{\text{ext}} + \boldsymbol{\nu} \\ \gamma_{\phi} \dot{\phi} &= -(-\nabla^{2})^{\mathfrak{a}} \frac{\delta \mathcal{H}}{\delta \phi} + \eta^{(\mathfrak{a})} \\ \mathcal{H}_{\text{int}} &= -\lambda \int d^{d} \mathbf{x} \, \phi(\mathbf{x}) V(\mathbf{x} - \mathbf{Y}) \\ \text{Demery, Dean. PRL (2010), PRE (2011).} \end{split}$$

- Optimal dragging simple problem to study thermodynamically optimal processes
- Memory effects (correlations in environment) strongly affect optimal dragging strategy
- Symmetry as universal feature of dragging problem (for linear processes)

Loos et al., Physical Review X 14, 021032 (2024) Garcia-Millan*, Schuettler*, Cates, Loos, ArXiv:2407.18542 (2024) Schuettler, Garcia-Millan, Cates, Loos, ArXiv:2501.18613 (2025)

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Conclusions

