

REPORT DOCUMENTATION PAGE			Form Approved OMB NO. 0704-0188		
The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA, 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.					
1. REPORT DATE (DD-MM-YYYY) 31-08-2018		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 13-Sep-2017 - 12-Jun-2018	
4. TITLE AND SUBTITLE Final Report: Non-equilibrium Statistical Mechanics and Curvature			5a. CONTRACT NUMBER W911NF-17-1-0429		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER 611102		
6. AUTHORS			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAMES AND ADDRESSES University of California - Irvine 141 Innovation Drive, Suite 250 Irvine, CA 92697 -7600			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211			10. SPONSOR/MONITOR'S ACRONYM(S) ARO		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S) 71222-MA-II.10		
12. DISTRIBUTION AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.					
13. SUPPLEMENTARY NOTES The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			Tryphon Georgiou
					19b. TELEPHONE NUMBER 949-824-9966

RPPR Final Report
as of 04-Sep-2018

Agency Code:

Proposal Number: 71222MAIL

Agreement Number: W911NF-17-1-0429

INVESTIGATOR(S):

Name: Tryphon Georgiou
Email: tryphon@uci.edu
Phone Number: 9498249966
Principal: Y

Organization: **University of California - Irvine**

Address: 141 Innovation Drive, Suite 250, Irvine, CA 926977600

Country: USA

DUNS Number: 046705849

EIN: 952226406

Report Date: 12-Sep-2018

Date Received: 31-Aug-2018

Final Report for Period Beginning 13-Sep-2017 and Ending 12-Jun-2018

Title: Non-equilibrium Statistical Mechanics and Curvature

Begin Performance Period: 13-Sep-2017

End Performance Period: 12-Jun-2018

Report Term: 0-Other

Submitted By: Tryphon Georgiou

Email: tryphon@uci.edu

Phone: (949) 824-9966

Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 0

STEM Participants: 0

Major Goals: The motivation for the work has been to obtain Landauer-type limits for information processing by real-life (engineering or biological) systems. Additional motivation from an engineering standpoint is the desire to design optimal and robust control schemes to effect transition of thermodynamic systems (possibly of interacting particles) between target states. The project aimed to quantify the cost of transitions in geometric terms, and obtain bounds for least amount of work required for such transitions.

Accomplishments: The goal has been to obtain quantitative estimates for the dissipation in the transference of a thermodynamic systems between states, in finite time. In particular, it is of interest to determine the least amount of energy that needs to be dissipated for such a transition. The research concluded with a very precise and elegant analytical results for the sought problem. More specifically, the main conclusion is that the work dissipated during a transition of thermodynamic system between two states depends on the control protocol (e.g., time-varying controlling potential) and it is precisely the length of a curve in the infinite dimensional space of probability distributions that the state (i.e., distribution) of the thermodynamic system traverses during the transition.

The derivation is quite general, for multivariable systems, and underscores the geometric nature non-equilibrium thermodynamic transitions. In particular, it shows that dissipation is measured by curve length in the so-called Wasserstein space, where the metric (Wasserstein metric) between probability distributions is the one inherited by Monge-Kantorovich optimal mass transport.

The accomplished goal, in particular, provides a precise formula for the least amount of "wasted energy" that is required for a thermodynamic transition over a specified time window.

Besides thermodynamics, application areas that stand to gain from the obtained results include nano-manipulation of materials, molecular motors, and in general, systems where stochastic excitation is substantial and energy dissipation is required to be kept low.

Training Opportunities: Nothing to Report

RPPR Final Report as of 04-Sep-2018

Results Dissemination: 7 regular journal refereed articles

1 book chapter

1 regular journal refereed article submitted

Matrix Optimal Mass Transport: a Quantum Mechanical Approach, Y. Chen, T.T. Georgiou, and A. Tannenbaum, IEEE Transactions on Automatic Control, August 2018, vol. 63 (8): pages 2612-2619; DOI 10.1109/TAC.2017.2767707

Vector-Valued Optimal Mass Transport Y. Chen , T.T. Georgiou, and Allen Tannenbaum, SIAM Journal on Applied Mathematics, 2018, vol. 78, No. 3 : pp. 1682-1696, DOI 10.1137/17M1130897

Steering the Distribution of Agents in Mean-Field Games System, Y. Chen, T. T. Georgiou, and M. Pavon, Journal of Optimization Theory and Applications, August 2018, DOI 10.1007/s10957-018-1365-7

Dynamic Relations in Sampled Processes, T.T. Georgiou and A. Lindquist, IEEE Control Systems Letters, January 2019, vol. 3(1): pages 144-149; DOI 10.1109/LCSYS.2018.2859481

An Efficient Algorithm for Matrix-Valued and Vector-Valued Optimal Mass Transport, Y. Chen, E. Haber, K. Yamamoto, T.T. Georgiou, A. Tannenbaum, Journal of Scientific Computing (2018): 1-22, DOI 10.1007/s10915-018-0696-8

Efficient Robust Routing for Single Commodity Network Flows, Y. Chen, T.T. Georgiou, M. Pavon, and A. Tannenbaum, IEEE Transactions on Automatic Control 63.7 (2018), DOI 10.1109/TAC.2017.2763418

M. Pouryahya, J.H. Oh, J.C. Mathews, J.O. Deasy, A.R. Tannenbaum, Characterizing Cancer Drug Response and Biological Correlates: A Geometric Network Approach. Scientific reports. 2018 Apr 23;8(1):6402, DOI 10.1038/s41598-018-24679-3

Wasserstein Geometry of Quantum States and Optimal Transport of Matrix-Valued Measures, Y. Chen, T.T. Georgiou and A. Tannenbaum, in Emerging Applications of Control and Systems Theory. Springer, 2018. Chapter 10, 139-150. DOI 10.1007/978-3-319-67068-3_10

Stochastic control and non-equilibrium thermodynamics: fundamental limits, Y. Chen, T.T. Georgiou and A. Tannenbaum, IEEE Transactions on Automatic Control, submitted.

Honors and Awards: 1) Tryphon Georgiou elected Fellow of the International Federation of Automatic Control, 2017

2) Tryphon Georgiou received the G.S. Axelby Outstanding Paper Award, 2017 by the IEEE Control Systems, December 2017

3) Allen Tannenbaum was a Keynote (Plenary) Speaker at SIAM Annual Conference in Control, 2017

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Co-Investigator

Participant: Allen Tannenbaum

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

RPPR Final Report
as of 04-Sep-2018

Participant Type: Graduate Student (research assistant)

Participant: Zahra Askarzadeh

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Rui Fu

Person Months Worked: 3.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Non-equilibrium Statistical Mechanics and Curvature

Tryphon T. Georgiou¹ and Allen R. Tannenbaum²

Abstract The project led to new insights on fundamental bounds on the work needed for far-from-equilibrium transitions. The motivation for the work has been to obtain Landauer-type limits for information processing by real-life (engineering or biological) systems. Additional motivation from an engineering standpoint is the desire to design optimal and robust control schemes to effect transition of thermodynamic systems (possibly of interacting particles) between target states. The project aimed to quantify the cost of transitions in geometric terms, and obtain bounds for least amount of work required for such transitions. Related advances and insights are reported on steering stochastic systems in transitioning between specified states – these include results on Gaussian mixture models, quantum systems and quantum evolutions of matrix-valued (i.e., non-commutative) probability distributions, systems with mean-field interaction, and stochastic evolutions on discrete spaces (robust routing of single commodity network flows). The report highlights the main results on the topic of thermodynamics which has been the driving concept of the funded project.

1. Forward

In recent years, it has become increasingly apparent across several fields that “far-from-equilibrium fluctuations are more interesting than one might have guessed (Jarzynski, 2011 [1]). Indeed, in statistical thermodynamics, Jarzynski’s Equality and Crook’s Fluctuation Theorem have opened up new ways to understand non-equilibrium thermodynamics, and new insights have been gained by focusing on the probability of trajectories of stochastically excited systems (thermodynamic ensembles). The basis for these developments has been a “large-deviations rationale” where minimizing the relative entropy between probability laws on path spaces of thermodynamic systems provides an organizing principle—a concept going back almost half a century to E.T. Jaynes. In fact, even earlier, the effect of large fluctuations on observed statistics of thermodynamic systems was considered by Erwin Schrödinger in 1931/32, in an attempt to explain quantum mechanics as a consequence of random classical fluctuations. More recently, several recent authors, including the PIs, sought to understand such thermodynamic transitions via stochastic control techniques via a deep link between work and relative entropy of between probability laws that dictate the randomness under different transition control protocols. It is this circle of ideas and tools that laid out the ground for this project.

The aim of the project has been to understand and quantify the cost of thermodynamic transitions and explain the character of fluctuation-dissipation relations in geometric terms. More specifically, probability

¹Department of Mechanical and Aerospace Engineering, University of California, Irvine, CA, USA

²Departments of Computer Science and Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY, USA

laws can be seen as points in the so-called Wasserstein space $\mathcal{P}_2$ – an infinite dimensional metric space equipped that resembles a Hilbert manifold. Thermodynamic transitions can now be seen as paths in this metric space, and the cost of transference between states can be quantified in terms of its length in the Wasserstein metric (W_2). As it turns out, there is a deep and, at the same time, precise connection between distances between probability distributions (with finite second order moments, i.e., in $\mathcal{P}_2$) and the relative entropy between the two. Thus, probabilistic and information theoretic concepts acquire geometric significance.

In this project we sought to explore the connection between thermodynamics, more specifically, work performed by stochastic particles and Wasserstein geometry, in order to quantify the energy cost of a transition under a specified control protocol as well as the optimal (minimal) cost for transition between thermodynamic states. These contributions are detailed in [2].

2. Statement of the problem studied

We consider damped stochastic systems in a controlled (time-varying) quadratic potential and study their transition between specified Gibbs-equilibria states in finite time. By the second law of thermodynamics, the minimum amount of work needed to transition from one equilibrium state to another is the difference between the Helmholtz free energy of the two end-point states and can only be achieved by a reversible (infinitely slow) process. We sought to compute the minimal gap between the work needed in a finite-time transition and the work during a reversible one. We also sought to compute the required work for transitions in the case of multidimensional systems, i.e., having a state-vector of high dimension. Under this general model, stochastic particles of thermodynamic ensemble are thought to obey the stochastic differential equation

$$dx(t) = -Q(t)x(t)dt + \sigma dw(t), \quad x(0) = x_0, \quad (1)$$

with $x \in \mathbb{R}^n$ and w a standard ($\mathbb{R}^n$ -vector-valued) Wiener process representing a thermal bath of temperature T ; the parameter

$$\sigma = \sqrt{2k_B T}.$$

This in fact is a vector-valued Ornstein-Uhlenbeck process. Here k_B is the Boltzmann constant [3], the Hookean force field $-Q(t)x(t)$ is the gradient of a time-varying quadratic Hamiltonian

$$\mathbf{H}_t(x) = \mathbf{H}(t, x) = \frac{1}{2}x'Q(t)x, \quad (2)$$

and the controlled parameter $Q(t) = Q(t)'$, $t \in [0, t_f]$, is scheduled so as to steer the system from a specified initial distribution for x_0 , to a final one for x_f , over the specified time window. The random variables x_0, x_f are taken to be Gaussian with zero mean and covariances Σ_0, Σ_f , respectively. That is, the distributions of the state at the two end points have probability densities are $\rho_0 = \mathcal{N}(0, \Sigma_0)$, $\rho_f = \mathcal{N}(0, \Sigma_f)$, or more explicitly,

$$\rho_i(x) = \frac{1}{(2\pi)^{n/2}|\Sigma_i|^{1/2}} e^{-\frac{1}{2}x'\Sigma_i^{-1}x}, \quad i \in \{0, f\},$$

and we seek to determine the minimum amount of work needed to effect the transition.

From a controls perspective, the problem amounts to *covariance control* of *bilinear* systems. Indeed, the dynamics are driven by the product of the control input $Q(t)$ times the state $x(t)$. By adjusting the

quadratic potential, it is possible to steer the system from one Gaussian distribution to another in finite time t_f . When this is the case, we are interested in the optimal control strategy $(Q(t), t \in [0, t_f])$ that minimizes the required control energy.

2. Background to the problem statement

It is well known that the minimum control energy must be greater than the Helmholtz free energy difference $\Delta\mathbb{F}$ between the two states (second law of thermodynamics). The important element in the problem formulation is the emphasis on the transition taking place over a finite interval $[0, t_f]$, hence it falls within the context of non-equilibrium thermodynamics.

Starting with the works by Jarzynski [4, 3] and Crooks [5], new insights began to shed light on the precise amount of work required for such finite-time transitions. Most famously, the Jarzynski equality

$$e^{-\beta\Delta\mathbb{F}} = \mathbb{E}\{e^{-\beta\mathbb{W}}\}, \quad (3)$$

relates the *equilibrium quantity* $\Delta\mathbb{F}$ (free energy difference between equilibrium states) to an *averaged non-equilibrium quantity* (exponential of the work; see our discussion below) over possible trajectories of the system in any finite-time transition. Throughout, $\mathbb{E}\{\cdot\}$ denotes the expectation on the path space of system trajectories and

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

where again T represents temperature of the heat bath and k_B the Boltzmann constant; β has units of “inverse-work.” The Jarzynski identity holds for arbitrary time-dependent driving force and not necessarily gradient of a quadratic potential. This type of result has led to a number of so-called *Fluctuation Theorems* in the literature, some of which have profound implications in biology and medicine [6, 7, 8].

Although the Jarzynski equality is quite remarkable, it doesn’t provide an explicit gap between the free energy difference $\Delta\mathbb{F}$ and the average work $\mathbb{W} = \mathbb{E}\{\mathbb{W}\}$. This gap is essential if we would like to find an optimal strategy with minimum work to move a thermodynamical system from one state to another. Following up on the Jarzynski equality, the authors of [9, 10] analyze the minimum energy control problems in the cases of a Brownian particle dragged by a harmonic optical trap through a viscous fluid, and of a Brownian particle subject to an optical trap with time dependent stiffness, in both overdamped and underdamped setting. Further, in [11, 12], the authors provide an optimal solution that relates the work dissipation to a Wasserstein distance. It can be viewed as a stronger version of the Second Law of Thermodynamics for certain Langevin stochastic processes in finite-time.

The present project and the work that has been carried out relates to the work in [11, 12] as well as in [9, 10]. Compared to [11, 12], our approach gives a control-theoretic account to the fluctuation type results in the case for Gaussian distributions. In addition, we provide an alternative proof for general cases with connections to the gradient flows with respect to the Wasserstein geometry [13]. The major difference to [9, 10] is that we consider the general multivariable case.

3. Summary of most important results

We begin by providing a brief account on Monge-Kantorovich Optimal Mass Transport (OMT) so as to introduce needed notation and concepts. We refer the reader to [14] for complete details as well as historical

background and modern applications of the relevant theory. The significance of OMT in nonequilibrium thermodynamics stems from the fact that energy dissipation appears to be captured in geometric terms by a concept of length that OMT provides for “curves” in the space of probability distributions, i.e., parameterized families of probability distributions that characterize the state trajectory of a thermodynamic system.

3a. Optimal mass transport

Consider two probability measures ρ_0, ρ_1 on $\mathbb{R}^n$. In the Kantorovich’s formulation of OMT with quadratic cost, one seeks a joint distribution $\pi \in \Pi(\rho_0, \rho_1)$ on $\mathbb{R}^n \times \mathbb{R}^n$, referred to as “coupling” of ρ_0 and ρ_1 , that minimizes the total cost, and so that the marginals along the two coordinate directions coincide with ρ_0 and ρ_1 , respectively, that is,

$$\inf_{\pi \in \Pi(\rho_0, \rho_1)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|^2 \pi(dxdy). \quad (4)$$

OMT has also an elegant stochastic control formulation, which reads as

$$\inf_u \mathbb{E} \left\{ \int_0^1 \|u(t, x(t))\|^2 dt \right\} \quad (5a)$$

$$\dot{x}(t) = u(t, x(t)) \quad (5b)$$

$$x(0) \sim \rho_0, \quad x(1) \sim \rho_1. \quad (5c)$$

This amounts to seeking a feedback control strategy (i.e., control u that is a function of the state x) requiring minimum energy that drives the state of an integrator from an initial probability distribution ρ_0 to a terminal probability distribution ρ_1 , through a path of distribution ρ_t , for $t \in [0, t_f]$.

Both of the above problems have unique solutions under the assumption that the marginal distributions are absolutely continuous. The square root of the minimum of the cost ((4) or (5)) defines a Riemannian metric on $P_2(\mathbb{R}^n)$, the space of probability distributions on $\mathbb{R}^n$ with finite second-order moments. This metric is known as the *Wasserstein metric* W_2 [13, 15, 14, 16]. On this Riemannian-type manifold, the geodesic curve connecting ρ_0 and ρ_1 is given by ρ_t , the probability density of $x(t)$ under the optimal control policy. This is called *displacement interpolation* [17] and it satisfies

$$W_2(\rho_s, \rho_t) = (t - s)W_2(\rho_0, \rho_1), \quad 0 \leq s < t \leq 1. \quad (6)$$

When the marginals ρ_0, ρ_1 are Gaussian distributions, the problem has a closed-form solution [18, 19, 20].

3b. Main results: least dissipation control

We consider the stochastic dynamical system in (1). As mentioned earlier, it represents a thermodynamical system with a quadratic Hamiltonian (2), overdamped and attached to a heat bath that is modeled by the stochastic excitation dw . The initial state is a Gaussian random vector $x_0 \sim \mathcal{N}(0, \Sigma_0)$, i.e., one having covariance Σ_0 and mean $\mathbb{E}\{x_0\} = 0$. The initial distribution is usually taken to be the stationary distribution with potential remaining constant on $(-\infty, 0]$ by keeping $Q(t) \equiv Q_0$ over $t \in (-\infty, 0]$, in which case $Q_0 = \frac{\sigma^2}{2} \Sigma_0^{-1}$, but this assumption is not required. We are interested in steering the state to the terminal distribution $\mathcal{N}(0, \Sigma_f)$ through selecting an optimal (least energy) time-varying control matrix variable $Q(\cdot) = Q'(\cdot)$ satisfying the boundary conditions $Q(0) = Q_0$, $Q(t_f) = Q_f$.

The control energy (work) delivered to the system along any particular sample path $x(\cdot)$ by the time-varying potential (2) is

$$\mathbf{W}(Q, x) := \int_0^{t_f} \frac{\partial \mathbf{H}(t, x)}{\partial t} dt = \int_0^{t_f} \langle \dot{Q}(t), \frac{\partial \mathbf{H}(t, x)}{\partial Q} \rangle dt,$$

where $\langle X, Y \rangle = \text{tr}(X'Y)$. Thus, by averaging over all possible sample paths, we obtain

$$\begin{aligned} \mathbb{W} &:= \mathbb{E}\{\mathbf{W}(Q, x)\} = \mathbb{E}\left\{\int_0^{t_f} \langle \dot{Q}, \frac{\partial \mathbf{H}}{\partial Q} \rangle dt\right\} \\ &= \mathbb{E}\left\{\int_0^{t_f} \frac{1}{2} \langle \dot{Q}(t), x(t)x(t)' \rangle dt\right\} \\ &= \frac{1}{2} \int_0^{t_f} \langle \dot{Q}(t), \Sigma(t) \rangle dt. \end{aligned}$$

Here, $\Sigma(\cdot)$ is the state covariance which, according to standard linear systems theory, evolves according to the Lyapunov equation

$$\dot{\Sigma}(t) = -Q(t)\Sigma(t) - \Sigma(t)Q(t) + \sigma^2 I. \quad (7)$$

The control which consist in selecting $Q(\cdot)$ may be discontinuous, reflecting instantaneous changes in the Hamiltonian $\mathbf{H}$, in which case, the expression for the work becomes the Lebesgue-Stieltjes integral

$$\mathbb{W} = \frac{1}{2} \int_{0^-}^{t_f^+} \langle dQ(t), \Sigma(t) \rangle, \quad (8)$$

where $0^-, t_f^+$ represent limits from below and above, respectively, so as to account for the discontinuities. Thus, the fundamental problem we deal with is:

Problem 1. Determine a control law

$$\{Q(t) \mid t \in [0, t_f]\}$$

that minimizes (8) subject to (7),

and the boundary conditions $Q(0) = Q_0, Q(t_f) = Q_f, \Sigma(0) = \Sigma_0, \Sigma(t_f) = \Sigma_f$.

The following result has been obtained and detailed in [2].

Theorem: Problem 1 has a unique minimizer $Q_{\text{opt}}(\cdot)$ that is computed as follows:

(i) If $\Sigma_0 = \Sigma_f$, then $\mathbb{W}_{\min} = 0$ and

$$Q_{\text{opt}}(t) = \frac{\sigma^2}{2} \Sigma_0^{-1}, \quad \Sigma(t) = \Sigma_0, \quad \text{for all } t \in (0, t_f).$$

(ii) If $\Sigma_0 \neq \Sigma_f$, then

$$\mathbb{W}_{\min} = -\frac{\sigma^2}{4} \text{trace} \log(\Sigma_f \Sigma_0^{-1}) + \frac{1}{t_f} \text{trace}(\Sigma_0 + \Sigma_f - 2(\Sigma_0^{1/2} \Sigma_f \Sigma_0^{1/2})^{1/2})$$

and

$$\begin{aligned}
Q_{\text{opt}}(t) &= \frac{\sigma^2}{2} \Sigma(t)^{-1} - (\Lambda(0)^{-1} + tI)^{-1} \\
\Sigma(t) &= (\Lambda(0)^{-1} + tI) M^{-1} (\Lambda(0)^{-1} + tI), \\
\Lambda(0) &= \frac{1}{t_f} (-I + \Sigma_0^{-1/2} (\Sigma_0^{1/2} \Sigma_f \Sigma_0^{1/2})^{1/2} \Sigma_0^{-1/2}) \\
M &= \Lambda(0)^{-1} \Sigma_0^{-1} \Lambda(0)^{-1}.
\end{aligned}$$

We remark that the optimal control $Q(t)$ is a continuous function on $(0, t_f)$. The limit values at $t = 0, t_f$ are

$$Q(0^+) = \frac{\sigma^2}{2} \Sigma_0^{-1} + \frac{1}{t_f} (I - \Sigma_0^{-1/2} (\Sigma_0^{1/2} \Sigma_f \Sigma_0^{1/2})^{1/2} \Sigma_0^{-1/2})$$

and

$$Q(t_f^-) = \frac{\sigma^2}{2} \Sigma_f^{-1} + \frac{1}{t_f} (-I + \Sigma_0^{1/2} (\Sigma_0^{1/2} \Sigma_f \Sigma_0^{1/2})^{-1/2} \Sigma_0^{1/2})$$

respectively. These may not be consistent with the boundary conditions $Q(0) = Q_0, Q(t_f) = Q_f$, which dictates the discontinuities of the optimal control at $t = 0, t_f$. When both the initial and terminal states are stationary, namely, $Q_0 = \frac{\sigma^2}{2} \Sigma_0^{-1}, Q_f = \frac{\sigma^2}{2} \Sigma_f^{-1}$, such discontinuities go to zero as the length of time t_f goes to infinity.

More succinctly, the conclusions of the above theorem with regard to the minimal work that is needed for the transition can be expressed as follows.

Theorem: For arbitrary marginal distributions ρ_0, ρ_f , provided we are free to change the Hamiltonian in an arbitrary manner (not requiring it to be quadratic), the minimal work for a thermodynamic transition is given by

$$\mathbb{W}_{\min} = \Delta F + \frac{1}{t_f} W_2(\rho_0, \rho_f)^2.$$

More generally, for a control protocol that may not necessarily be optimal, the following holds.

Theorem:

$$\mathbb{W} = \Delta F + \frac{1}{t_f} (\text{length}_{W_2}(\{\text{path } \rho_t \mid t \in [0, 1]\}))^2,$$

where

$$\text{length}_{W_2}(\{\text{path } f_t \mid t \in [0, 1]\})$$

is the length of the curve $\{f_t \mid t \in [0, 1]\}$ in the Wasserstein space of probability distributions endowed with the Wasserstein metric.

Thus, “least-work” paths or, more precisely, “least-dissipation” paths correspond to geodesic flows in the Wasserstein space for the state (probability distribution) of a thermodynamic system. *This gives an interesting novel view of the Second Law of Thermodynamics in which dissipation is explicitly characterized in terms of a transport distance and geometry.*

To put the above statement in context, recall that for reversible processes, one has

$$\mathbb{W} = \Delta\mathbb{F},$$

while for general processes

$$\mathbb{W} \geq \Delta\mathbb{F}.$$

Such statements are equivalent to the second law of thermodynamics, which states that the total entropy of an isolated system is nondecreasing. The theorems above provide a stronger lower bound for entropy production of a finite-time process, and *this bound connects thermodynamics and optimal mass transport*. The difference $\mathbb{W} - \Delta\mathbb{F}$ is the entropy production, or *work dissipation*, and denoted $\mathbb{W}_{\text{diss}}$. The fundamental lower bound of work dissipation is

$$\mathbb{W}_{\text{diss}} \geq \frac{1}{t_f} W_2(\rho_0, \rho_f)^2,$$

and is valid for any (irreversible) process evolving in a finite time-interval $[0, t_f]$. The lower bound is achieved by the optimal protocol and the corresponding probability density flow is the displacement interpolation between ρ_0 and ρ_f . In our research publication [2], besides a detailed theoretical analysis and derivation of the results, we present examples of a laser trap of varying center or strength. Finally, the results also suggest a promising direction to solve constrained thermodynamical control problems.

4. Other research contributions related and supported by the grant

Work under the grant impacted ongoing research that culminated in original contributions that are highlighted below.

4a. Network robustness and control

Networks come in all shapes and forms –transportation, communication, power, gene regulatory networks, etc. [21]. Yet, one important universal and desirable quality is their ability (or lack thereof) to adapt and return to equilibrium in response to an external disturbance, or to structural and dynamic changes that may have taken place, while maintaining functionality [22]. One way to quantify “robustness,” following [23], is in terms of the rate function from large deviations theory. A key idea relies on the positive correlation between an increase of curvature and network functional robustness, a fact which may be regarded as a *geometric version of the Fluctuation Theorem* as formulated in [23]. Our ongoing work on network efficiency and robustness has led to the recent publication [24], detailing a probabilistic approach to obtaining efficient robust routing for a single commodity over a transportation network. Also in [25] we presented a study of how geometry of transport and a concept of curvature of graphs are applied to gene regulatory networks can characterize cancer drug response and guide therapy.

4b. Probability flows and control with mean-field interaction

In [26] we explored models of transport where particles/agents experience a mean-field type interaction. The presence of a mean field, or of more general types of interaction potential, may be used to model a variety of physical systems. In particular, little is known for thermodynamics of interacting particle systems and the minimal dissipation in thermodynamic transitions. The work in [26] represents a first attempt to grapple with relevant issues.

4c. Fundamentals of system identification

A fundamental problem is to identify linear dynamical relations that may exist between the components of a continuous-time vectorial process. What is typically available to engineers and scientists is the discrete-time sampled process (i.e., a time series) of measurements collected at a given finite sampling rate (possibly nonuniform). The study in [27] considers issues of statistical estimation and, in particular, how to identify the maximal number of dynamical dependencies between the entries of the process at the finest time scale. The key point that makes the result significant is that dynamical dependencies are masked at the level of the sampled process, and thereby, it is possible that system identification toolboxes miss the correct number of dynamical couplings between observed time series as those are obfuscated due to sampling. Modern-day applications, which aim towards high dimensional data and possibly varying sampling protocols, further underscore the importance of a careful consideration of how sampling affects dynamical dependencies. Particular applications to identifying dynamical links in networks between time series at different nodes, and as a consequence, the structure of the network, are discussed in [27].

References

- [1] C. Jarzynski, “Equalities and inequalities: irreversibility and the second law of thermodynamics at the nanoscale,” *Annu. Rev. Condens. Matter Phys.*, vol. 2, no. 1, pp. 329–351, 2011.
- [2] Y. Chen, T. Georgiou, and A. Tannenbaum, “Stochastic control and non-equilibrium thermodynamics: fundamental limits,” *arXiv preprint arXiv:1802.01271*, 2018.
- [3] C. Jarzynski, “Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach,” *Physical Review E*, vol. 56, no. 5, p. 5018, 1997.
- [4] —, “Nonequilibrium equality for free energy differences,” *Physical Review Letters*, vol. 78, no. 14, p. 2690, 1997.
- [5] G. E. Crooks, “Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences,” *Physical Review E*, vol. 60, no. 3, p. 2721, 1999.
- [6] U. Seifert, “Stochastic thermodynamics, fluctuation theorems and molecular machines,” *Reports on Progress in Physics*, vol. 75, no. 12, p. 126001, 2012.
- [7] R. Marsland and J. England, “Far-from-equilibrium distribution from near-steady-state work fluctuations,” *Phys. Rev. E*, vol. 92, no. 5, 2015.
- [8] R. Sandhu, T. Georgiou, E. Reznik, L. Zhu, I. Kolesov, Y. Senbabaoglu, and A. Tannenbaum, “Graph curvature for differentiating cancer networks,” *Scientific Reports*, vol. 5, p. 12323, 2015.
- [9] T. Schmiedl and U. Seifert, “Optimal finite-time processes in stochastic thermodynamics,” *Physical Review Letters*, vol. 98, no. 2, p. 108301, 2007.
- [10] A. Gomez-Marin, T. Schmiedl, and U. Seifert, “Optimal protocols for minimal work processes in underdamped stochastic thermodynamics,” *The Journal of Chemical Physics*, vol. 129, no. 2, p. 024114, 2008.

- [11] E. Aurell, C. Mejía-Monasterio, and P. Muratore-Ginanneschi, “Optimal protocols and optimal transport in stochastic thermodynamics,” *Physical Review Letters*, vol. 106, no. 25, p. 250601, 2011.
- [12] E. Aurell, K. Gawdzki, C. Mejía-Monasterio, R. Mohayaei, and P. Muratore-Ginanneschi, “Refined second law of thermodynamics for fast random processes,” *Journal of Statistical Physics*, vol. 147, no. 3, pp. 487–505, 2012.
- [13] R. Jordan, D. Kinderlehrer, and F. Otto, “The variational formulation of the Fokker–Planck equation,” *SIAM Journal on Mathematical Analysis*, vol. 29, no. 1, pp. 1–17, 1998.
- [14] C. Villani, *Topics in Optimal Transportation*. American Mathematical Soc., 2003, no. 58.
- [15] F. Otto, “The geometry of dissipative evolution equations: the porous medium equation,” *Communications in Partial Differential Equations*, 2001.
- [16] C. Villani, *Optimal Transport: Old and New*. Springer, 2008, vol. 338.
- [17] R. J. McCann, “A convexity principle for interacting gases,” *Advances in Mathematics*, vol. 128, no. 1, pp. 153–179, 1997.
- [18] A. Takatsu, “Wasserstein geometry of gaussian measures,” *Osaka Journal of Mathematics*, vol. 48, no. 4, pp. 1005–1026, 2011.
- [19] D. Dowson and B. Landau, “The fréchet distance between multivariate normal distributions,” *Journal of Multivariate Analysis*, vol. 12, no. 3, pp. 450–455, 1982.
- [20] X. Jiang, Z.-Q. Luo, and T. T. Georgiou, “Geometric methods for spectral analysis,” *IEEE Transactions on Signal Processing*, vol. 60, no. 3, pp. 1064–1074, 2012.
- [21] A.-L. Barabási, “The network takeover,” *Nature Physics*, vol. 8, no. 1, p. 14, 2011.
- [22] U. Alon, *An introduction to systems biology: design principles of biological circuits*. Chapman and Hall/CRC, 2006.
- [23] L. Demetrius and T. Manke, “Robustness and network evolution?an entropic principle,” *Physica A: Statistical Mechanics and its Applications*, vol. 346, no. 3-4, pp. 682–696, 2005.
- [24] Y. Chen, T. T. Georgiou, M. Pavon, and A. Tannenbaum, “Efficient robust routing for single commodity network flows,” *IEEE Transactions on Automatic Control*, vol. 63, no. 7, 2018.
- [25] M. Pouryahya, J. H. Oh, J. C. Mathews, J. O. Deasy, and A. R. Tannenbaum, “Characterizing cancer drug response and biological correlates: A geometric network approach,” *Scientific reports*, vol. 8, no. 1, p. 6402, 2018.
- [26] Y. Chen, T. T. Georgiou, and M. Pavon, “Steering the distribution of agents in mean-field games system,” *Journal of Optimization Theory and Applications*, pp. 1–26, 2018.
- [27] T. T. Georgiou and A. Lindquist, “Dynamic relations in sampled processes,” *IEEE Control Systems Letters*, vol. 3, no. 1, pp. 144–149, 2019.