Information Engines at the Frontiers of Nanoscale Thermodynamics

Organizing Committee:
James Crutchfield
Korana Burke
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July 25 – August 2, 2019

Telluride Intermediate School, 725 W Colorado Ave Telluride, CO 81435

Contents

1 Scope

Synthetic nanoscale machines, like their macromolecular biological counterparts, perform tasks that involve the simultaneous manipulation of energy, information, and matter. In this they are information engines systems with two inextricably intertwined characters. The first aspect, call it physical, is the one in which the system is seen embedded in a material substrate that is driven by, manipulates, stores, and dissipates energy. The second aspect, call it informational, is the one in which the system is seen in terms of its spatial and temporal organization generates, stores, loses, and transforms information. Information engines operate by synergistically balancing both aspects to support a given functionality, such as extracting work from a heat reservoir. Recent years witnessed remarkable progress in the theoretical understanding and experimental exploration of how physical systems compute, process, and transfer information. We are on the verge of a synthesis that will allow us to account for a new thermodynamics of information. As we continue to develop a deeper understanding of the world around us, the fundamental question arises, How does nature compute? Numerous researchers, both theorists and experimentalists, are working towards understanding how information is transferred through and transformed at the nanoscale – with applications ranging from biological systems to quantum devices. The aim of this workshop is to exchange ideas from research in Nonequilibrium Thermodynamics, Classical and Quantum Information, Statistical Mechanics, Biophysics, and Nonlinear Dynamics. These questions are relevant in a wide variety of fields including Nanoscale Statistical Mechanics, Finite-Time Thermodynamics, Quantum Thermodynamics, Quantum Computation, Quantum Communication, Quantum Optimal Control Theory, and Biological Physics.

2 Program

2.1 Overview

Useful information:

- The workshop is organized around stimulating discussion and sharing ideas. The schedule is relaxed. Talks are only in the mornings, leaving the afternoons free for work, discussions, and recreation. There are also a number of evening events, from group dinners to the BBQ and a community talk that bring us back together.
- Some useful area maps are provided at the end of this Program.
- The abstract have been sorted according to topics, and we will have sessions on *thermodynamics of information, information engines and Maxwell demons, quantum thermodynamics and quantum information, stochastic thermodynamics, quantum and nanotechnologies, entropy production and thermodynamic cost*, and *thermodynamic control and optimal processes*.
- We will have no sessions on Sunday, but the meeting rooms will be available.
- Breakfast and lunch will be served at the Telluride Intermediate School. However, there is **NO** breakfast or lunch on Sunday.
- The session chairs will observe the Frauenfelder rules:

  > Hans Frauenfelder is the inventor of the "Frauenfelder Rules", which provide a guideline about the most successful way to run a seminar at a research workshop, according to which a presentation should take up no more than 66% of the allotted time, the rest being used for questions and in-depth discussion.

  So, please make sure that your presentation is at most 30 mins, which leaves at least 10 mins for discussion.

	Thursday 07/25	Friday 07/26	Saturday 07/27	Sunday 07/28	Monday 07/29	Tuesday 07/30	Wednesday 07/31	Thursday 08/01	Friday 08/02
8:20	breakfast	breakfast	breakfast		breakfast	breakfast	breakfast	breakfast	breakfast
9:00	opening	**Menges**	**Jarzynski**		**Chamberlin**	**Sahu**	**Pal**	**Lu**	**Hodson**
9:40	**Crutchfield**	**Loomis**	**Wimsatt**		**Šafránek**	**Elenewski**	**Brito**	**Rahav**	**Hinczewski**
10:20	coffee	coffee	coffee		coffee and picture	coffee	coffee	coffee	coffee
11:00	**Rupe**	**Deffner**	**Jurgens**		round table	**Zwolak**	Tutorial	Tutorial	**Boyd**
11:40	**Roukes**	**Myers**	**Ray**		round table	**Anza**	Tutorial	Tutorial	Closing
12:20	lunch	lunch	lunch		lunch	lunch	lunch	lunch	lunch
13:00									
13:40									
14:20									
15:00									
15:40									
16:20									
17:00									
17:40	group dinner				group dinner	town talk	TSRC bbq		
18:20							TSRC bbq		
19:00							TSRC bbq		

2.2 Thursday, July 25, 2019: Thermodynamics of computation

8:20 am – 9:00 am: Badge Pick-Up & Breakfast at TSRC

Check-In and breakfast at the Telluride Intermediate School

Session Chair: **KORANA BURKE**

9:00 am – 9:40 am: Opening talk

James P. Crutchfield
Korana Burke
Sebastian Deffner

9:40 am – 10:20 am: Thermodynamic Computing: Fast, Cheap, and Under Control

James P. Crutchfield
University of California, Davis

The paradigm of thermodynamic computing has arrived, driven by recent theoretical and experimental progress, pitched to circumvent the end of Moore's multi-decadal exponential progress in computing speed and density, and offered as a complement to quantum computing. I will review a recent planning effort (Computing Community Consortium, January 2019, Honolulu) aimed to accelerate reducing our recent progress to practice. As part of this I will also give a rather synoptic and optimistic survey of that progress, somewhat biased to the outputs from our multiyear Information Engines workshop series. Looking forward, I will address several open challenges. The first is to understand how the recent progress was built out of a calculus of limitations—from deterministic unpredictability, quantum uncertainty, undecidability, and uncomputability to our current inability to track the flow of information, identify causal mechanisms, define structural complexity, and converge on unique explanatory models. What new limitations and innovations can we anticipate? The second challenge is to unpack what Landauer meant by "information-bearing degrees of freedom". Explicitly addressing this is key to an objective theory of physical computing. The final challenge is what I call Landauer's Stack: What are the actual thermodynamic costs of information processing? If we add up currently-identified thermodynamic costs – Landauer erasure, Information Processing Second Law, synchronization and error correction, implementation modularity, high reliability, and the like – can we accurately predict the energetics of contemporary and future computing? If not, how far are we from doing so and what might we be missing?

10:20 am – 11:00 am: Coffee break

11:00 am – 11:40 am: Discovering Unknown Physics: Models, Mechanism, and the Computation Dynamics Duality

Adam Rupe
University of California, Davis

When confronted with an as-of-yet unexplained phenomenon the usual approach is to design a parametric model as a mechanistic hypothesis explaining the phenomenon. A minimal model that distills the essence of the new phenomenon must capture key underlying mechanisms. Creating such a model, however, is highly non-trivial and distilled models can lead to misleading predictions. More troubling, for sufficiently complex systems such a distillation is not possible. Quite "large" complicated models may be required to produce requisite details of the phenomenon, and the simulated output of such models is effectively as complex as the natural phenomenon. Even for simpler models, the disconnect between model and the resulting emergent phenomenon renders the model an unsatisfactory mechanistic explanation. To make progress, I will discuss a useful duality between computation theory and complex dynamical systems, and then describe my recent work extending the computational mechanics framework for studying physical spatiotemporal systems. The move from parametric system-of-equation modeling to nonparametric computation-theoretic models allows for automated discovery of minimal models that capture structurally relevant components of the system. However, deducing physically-interpretable mechanisms from these models is an open challenge. Drawing on the computation-dynamics duality, I will suggest low-dimensional computational mechanics as a promising path towards uncovering physical and causal mechanisms.

11:40 am – 12:20 pm: Emerging experimental approaches for studying information engines

Michael Roukes
Caltech

Flux qubits and nanomechanical resonators provide rich and unique experimental platforms for studying the physics of information coupled to energy transport and dissipation at the nanoscale. Emerging capabilities for single-phonon measurement and control offer unprecedented opportunities for interrogating these experimental platforms. In my presentation I'll provide a succinct review of these exciting prospects, as well as the rather significant technological challenges we are facing in our efforts to implement them.

This work is being carried out in close collaboration with theorists Jim Crutchfield and Mark Dykman, and, on the experimental side, with Jukka Pekola (Aalto U.), Chiara Dario (Caltech), Matt Matheny (Caltech), Olli-Pentti Saira (BNL), and M. Selim Hanay (Bilkent U.)

12:20 pm – 01:00 pm: Lunch

5:40 pm: Group dinner at the Tent behind Telluride Intermediate School

2.3 Friday, July 26, 2019: Quantum thermodynamics

8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

Session Chair: **JAMES P. CRUTCHFIELD**

9:00 am – 9:40 am: Nanoscale Thermometry and Quantized Heat Transport

Fabian Menges
University of Colorado, Boulder

Thermal energy transfer and dissipation can influence the physical properties of matter, control the kinetics of chemical reactions, and trigger bio-molecular mechanisms in living organism. Understanding the thermodynamic roots of physical processes is therefore one of the key challenges in the natural sciences, in particular for systems with characteristic length and time scales comparable to or even shorter than the mean free path and relaxation times of energy carriers such as electrons and phonons

Here, we will review recent experimental approaches to characterize local energy transfer and dissipation processes based on scanning probe microscopy and micro-electromechanical calorimeters (MEMS) with integrated temperature sensors. Based on numerous examples, we will illustrate how scanning probe thermometry enables the real-space quantification of Joule and Peltier effects in operating nanoelectronic devices down to 10 nm spatial and tens of pico-Watt heat flux resolution. In addition, we will discuss the study of heat transport across molecules and atomic-scale contacts, ultimately demonstrating the validity of fundamental charge and heat transfer relations down to the limit of single thermal conductance quanta. Finally, we will provide an outlook on our developments of energy and time-resolved photo-thermal scanning probe techniques, as well as their potential to unravel thermodynamic processes in optical nanocavities.

9:40 am – 10:20 am: Quantum memory compression and thermodynamic efficiency

Samuel Loomis
University of California, Davis

Quantum coherence allows for smaller-memory generators of classical processes, called q-machines. We examine the challenges and implications of placing q-machines in the thermodynamic context of a quantum information engine with a classical information reservoir. Using the formalism of thermal operations and majorization, we compute the minimal work cost of the quantum engine overall, and then consider additional costs due to modularity. We show that, when modularity is considered, information engines which utilize quantum coherence for memory compression cannot be perfectly efficient, and their dissipation grows with the amount of compression achieved.

10:20 am – 11:00 am: Coffee break

11:00 am – 10:40 am: Efficiency of harmonic quantum Otto engines at maximal power

Sebastian Deffner
UMBC

Recent experimental breakthroughs produced the first nanoheat engines that have the potential to harness quantum resources. An instrumental question is how their performance measures up against the efficiency of classical engines. For single ion engines undergoing quantum Otto cycles it has been found that the efficiency at maximal power is given by the Curzon-Ahlborn efficiency. This is rather remarkable as the Curzon-Alhbron efficiency was originally derived for endoreversible Carnot cycles. Here, we analyze two examples of endoreversible Otto engines within the same conceptual framework as Curzon and Ahlborn's original treatment. We find that for endoreversible Otto cycles in classical harmonic oscillators the efficiency at maximal power is, indeed, given by the Curzon-Ahlborn efficiency. However, we also find that the efficiency of Otto engines made of quantum harmonic oscillators is significantly larger.

11:40 am – 12:20 pm: Bosons outperform Fermions – the thermodynamic advantage of symmetry

Nathan Myers
UMBC

The recent miniaturization of heat engines to the nanoscale introduces the possibility of engines that harness quantum resources. The analysis of quantum engines provides important insight into how their efficiency compares to classical analogues and deepens our understanding of thermodynamic mechanisms at the quantum scale. We examine a quantum Otto engine with a harmonic working medium consisting of two non-interacting particles to explore the use of wave function symmetry as an accessible quantum resource. The efficiency and power outputs are compared based on whether the medium consists of bosons or fermions. We show that the bosonic system displays enhanced performance when compared to two single particle engines, while the fermionic system displays reduced performance. We explore the trade-off between efficiency and power output and show that the system with the best trade-off value depends on the ratio of bath temperatures. We also examine the parameter regimes under which the system functions as engine, refrigerator, or heater and demonstrate that the bosonic system operates under a wider parameter space both when operating as an engine and as a refrigerator.

Joint work with Priyo Shankar Pal and Sebastian Deffner.

12:20 pm – 01:00 pm: Lunch

2.4 Saturday, July 27, 2019: Thermodynamic control I

8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

Session Chair: **SEBASTIAN DEFFNER**

9:00 am – 9:40 am: Quantum Impulse Control

Chris Jarzynski
University of Maryland, College Park

The quantum adiabatic theorem governs the evolution of a wavefunction under a slowly time-varying Hamiltonian. I will consider the opposite case of a Hamiltonian that is varied impulsively: an infinitely strong perturbation $U(x,t)$ is applied over an infinitesimal time interval, of duration epsilon. When the strength of the perturbation scales like $1/\epsilon^2$, an interesting dynamical behavior emerges, characterized by an abrupt displacement of the wave function in coordinate space. I will solve for the evolution of the wavefunction in this situation. Remarkably, the solution involves a purely classical construction, yet describes the quantum evolution exactly, rather than (small-$\hbar$) approximately. I will use these results to show how appropriately tailored impulses can be used to control the behavior of a quantum wavefunction.

9:40 am – 10:20 am: Boxed Protocols: The Well-Tempered Cannonball

Gregory Wimsatt
University of California, Davis

Many results in small-scale non-equilibrium thermodynamics can be applied to a particular form of model universe: a small system under study (SUS) evolves while in contact with both a laboratory device and thermal environment. While both the lab device and thermal environment thus contribute to the dynamics for the SUS' evolution, we assume that we can prepare the lab device to instantiate a predetermined time-dependent contribution called the protocol. But the stochastic contribution due to the thermal environment allows for many possible SUS microstate trajectories. Then since each SUS microstate presents a different instantaneous contribution to the exact dynamics for the lab device, the assumption that a single specific predetermined protocol can be elicited from the lab device is questionable. I explore this issue by simulating a simple "boxed" protocol. I simulate a 1D SUS and 1D toy lab device coupled via a particular 2D potential under Langevin dynamics. With appropriate choice of parameters, a properly initialized lab device can then evolve nearly deterministically and guarantee an effective protocol for the SUS. Despite the lack of strict determinism in the effective protocol, I apply several fluctuation theorems that apply for true protocols and find agreement with the results of the simulation.

10:20 am – 11:00 am: Coffee break

11:00 am – 11:40 am: Exact Functional Thermodynamics For Arbitrary Maxwellian Demons

Alexandra Jurgens
University of California, Davis

Autonomous Maxwellian demons use structured environments as a resource to generate work, randomizing ordered inputs and leveraging the increased Shannon entropy to transfer energy from a thermal reservoir to a work reservoir. To date, determining their functional thermodynamic operating regimes was restricted to information engines for which correlations among information-bearing degrees of freedom can be calculated exactly via compact analytical forms—a highly restricted set of engines. Despite information engines being represented as finite hidden Markov chains, the restriction arises since the processes generated are notoriously complicated. Even if finite state, (i) no finite expression for their Shannon entropy rate exists, (ii) the set of their predictive features is generically uncountably infinite, and (iii) their statistical complexity diverges. Attempting to circumvent these problems, previous entropy-rate calculations either heavily constrained Demon structure or invoked approximations that misclassify thermodynamic behavior or simply fail. Here, we adapt recent results from dynamical systems theory to efficiently and accurately calculate the entropy rates and the rate of statistical complexity divergence of general hidden Markov chains. The results precisely determine the thermodynamic functionality for previously-studied Maxwellian demons. This allows us to accurately characterize the thermodynamic operating regimes for finite-state Maxwellian demons with arbitrary numbers of transitions, as well as find the rate of statistical complexity divergence—the dimension of the minimal set of predictive features for the underlying thermodynamic process. Beyond markedly improving previous analyses and greatly expanding the class of analyzable information engine, the new methods allow for (i) automated surveys of information engines, (ii) discovering new kinds of engine functionality, and (iii) optimizing desirable engine properties.

Joint work with Alec Boyd, Jim Crutchfield, and Ariadna Venegas-Li.

11:40 am – 12:20 pm: Variations on a Demonic Theme

Kyle Ray
University of California, Davis

Szilard's now-famous single-molecule engine was only the first of three constructions he introduced in 1929 to resolve several paradoxes arising from Maxwell's demon. We analyze Szilard's remaining two demon models. We show that the second one, though a markedly different implementation employing a population of distinct molecular species and semi-permeable membranes, is informationally and thermodynamically equivalent to an ideal gas of the single-molecule engines. Since it is a gas of noninteracting particles one concludes, following previous work by Boyd and Crutchfield, that (i) it reduces to a chaotic dynamical system—called the Szilard Map, a composite of three piecewise linear maps that implement the thermodynamic transformations of measurement, control, and erasure; (ii) its transitory functioning as an engine that converts disorganized heat energy to work is governed by the Kolmogorov-Sinai entropy rate; (iii) the demon's minimum necessary "intelligence" for optimal functioning is given by the engine's statistical complexity, and (iv) it's functioning saturates thermodynamic bounds and so it is a minimal, optimal implementation. We show that Szilard's third model is rather different and addresses the fundamental issue, raised by the first two, of measurement in and by thermodynamic systems and entropy generation.

We give a complete thermodynamic and computational mechanics treatment, revealing the minimal measurement tasks that the first two engines require as an example of the Principle of Requisite Complexity. Taken together, Szilard's suite of constructions lays out a range of possible realizations of Maxwellian demons that anticipated by almost two decades Shannon's and Wiener's concept of information as surprise and cybernetics's notion of functional information.

12:20 pm – 01:00 pm: Lunch

2.5 Sunday, July 28, 2018: Free day

No program, no breakfast or lunch.

2.6 Monday, July 29, 2018: Fluctuations I

8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

Session Chair: **KORANA BURKE**

9:00 am – 9:40 am: Seeking a well-defined local temperature for nanoscale fluctuations

Ralph V. Chamberlin
Arizona State University

Temperature (T) should provide a unifying concept across all size scales, and methods of research. However, we find inconsistencies in the local T deduced from equilibrium fluctuations found in experiments, theory, and computer simulations. One example is our nonlinear spectroscopy measurements yielding heterogeneous values of local T, unlike the uniformity needed for standard thermal equilibrium. Another example is our MD simulations showing a static local T from average energies that accurately matches the equipartition theorem, while the dynamic local T from energy fluctuations often exceeds the textbook value, sometimes by more than a factor of fifty. Any viable definition of local T must strictly conserve total energy, even on the scale of nanometers, as fully formulated only by the laws of small-system thermodynamics ("nanothermodynamics"). I will discuss how various nonlinear corrections to Boltzmann's factor can improve the concept of local T in computer simulations and measured behavior. One approach utilizes physical information from Landauer's principle to maintain maximum entropy during equilibrium fluctuations.

9:40 am – 10:20 am: Extreme fluctuations of entropies in quantum systems

Dominik Šafránek
University of California, Santa Cruz

The intuition that we have about entropy – coming largely from the Boltzmann entropy – is that the maximum entropy state is very close to the equilibrium state, while low entropy is associated with highly non-equilibrium states. I this talk I will investigate two well-developed definitions of entropy relevant for describing the dynamics of isolated quantum systems, and ask if they lead to this same intuition, by studying their extreme fluctuations. We choose entanglement entropy, because it is very often used, and Observational entropy, which is a recently introduced generalization of Boltzmann entropy to quantum systems, for comparison. While entanglement entropy is an important measure that quantifies non-local correlations, we find that Observational entropy, which quantifies localization of particles instead, matches better with our intuition from the Boltzmann entropy.

10:20 am – 11:00 am: Coffee break and group picture

11:00 am – 12:20 pm: Round table: Thermodynamics of information – quo vadis?

12:20 pm – 01:00 pm: Lunch

5:40 pm : Group dinner at the Tent behind Telluride Intermediate School

2.7 Tuesday, July 30, 2019: Transport in nanosystems

8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

Session Chair: **JAMES P. CRUTCHFIELD**

9:00 am – 9:40 am: Bio-lite channels: Synthetic nanoscale pores for investigating ion selectivity and optimal transport

Subin Sahu
University of Maryland, College Park

Ionic transport through nanoscale pores and channels is a vital process for information exchange in physiology. For example, it generates the action potential necessary for electrical signaling between excitable cells such as neurons and muscle cells. The efficient signal transmission in neurons requires the channels to have both high ion specificity and high ion permeability. These two characteristics are at odds with each other. As well, the primary mechanism for ion selectivity in biological ion channels is still contentious, as several factors such as electrostatics, van der Waals forces, hydration, and fluctuations of the channel influence the transport. The structural complexities of these channels impede delineation of individual factors. However, biomimetic sub-nanoscale pores, such as the recently discovered graphene crown-ether, can elucidate the basic mechanisms of ionic transport as these pores are much simpler while retaining key aspects of the process. Similar to the biological pore, the completion between electrostatics and dehydration gives the landscape for ion transport through these synthetic pores. Moreover, a few picometer change in the pore size brings about a colossal change in the ionic current and can even change the transport mechanism. These sub-nanoscale, functionalized pores, therefore, give routes to developing a mechanistic understanding of ion transport in confined geometries with closely packed charged groups and thus illuminating the behavior of biological ion channels and synthetic pores a like.

1. S. Sahu, J. Elenewski, C. Rohmann, and M. Zwolak. "Optimal transport and colossal ionic mechano-conductance in graphene crown ether." Sci. Adv. **5**, eaaw5478 (2019)

2. S. Sahu and M. Zwolak. "Colloquium: Ionic phenomena in nanoscale pores through 2D materials." Rev. Mod. Phys. **91**, (2019)

9:40 am – 10:20 am: The Multiscale, Nonlinear Dynamics of Biomolecular Energy Redistribution

Justin Elenewski
University of Maryland, College Park

Although selective energy redistribution is critical to the function of numerous biomolecules and functional nanomaterials, the processes mediating these dynamics remain a poorly understood facet of nonequilibrium thermodynamics. In this talk, I will discuss how topological features, nonlinearities, and energy landscape architecture can collude to define biomolecular heat propagation. Our exhaustive all-atom simulations and novel local-in-time and space analysis - which is equally applicable to both theory and experiment - permit the multiscale dissection of energy migration in biomolecules. Unlike transport through small-molecule systems, we find that nonlinearity dominates over coherent processes at even at short length- and time-scales. Leveraging these observations, I will demonstrate how vibrational energy transport can probe otherwise inaccessible aspects of macromolecular dynamics and the interactions that underly biological function.

This work is a collaboration with Michael Zwolak (NIST) and Kirill Velizhanin (LANL).

10:20 am – 11:00 am: Coffee break

11:00 am – 11:40 am: Breaking the entanglement barrier: Tensor network simulation of quantum transport

Michael Zwolak
National Institute for Standards and Technology

The recognition that large classes of quantum many-body systems have limited – or efficiently representable – entanglement in the ground and low-lying excited states led to dramatic advances in their numerical simulation via so-called tensor networks. However, global dynamics elevates many particles into excited states, and can lead to macroscopic entanglement (seen both experimentally and theoretically) and the failure of tensor networks. Here, we show that for quantum transport – one of the most important cases of this failure – the fundamental issue is the canonical basis in which the scenario is cast: When particles flow through an interface, they scatter, generating a "bit" of entanglement between spatial regions with each event. The frequency basis naturally captures that – in the long time limit and in the absence of an inelastic event – particles tend to flow from a state with one frequency to a state of identical frequency. Recognizing this natural structure yields a striking – exponential in some cases – increase in simulation efficiency, greatly extending the attainable spatial and time scales. This approach enables the mapping of the conductance diagram of the paradigmatic Anderson impurity problem. The concepts here broaden the scope of tensor network simulation into hitherto inaccessible classes of non-equilibrium many-body problems.

11:40 am – 12:20 pm: Thermalization and Log-growth of local entanglement in MBL systems

Fabio Anza
University of California, Davis

In the past few years Many-Body Localization (MBL) has been established as a robust mechanism to avoid local thermalization in quantum systems. This makes them a promising platform for quantum computation, alternative to the usual one based on isolated QuBits. Despite the large body of results (1) experimental proof of the existence of MBL is still lacking and (2) we do not have a detailed understanding of the entanglement evolution for systems in the MBL phase. After a brief introduction to MBL, I will present a systematic study of the dynamics of entanglement between arbitrary partitions in the canonical model for MBL, and show that local measurements are sufficient to experimentally determine its existence.

12:20 pm – 01:00 pm: Lunch

06:00 pm – 07:00 pm: TSRC town talk – What flies can teach us about our kidneys

Aylin Rodan
University of Utah

Cash bar at 5:30 pm.

2.8 Wednesday, July 31, 2019: Fluctuations II

8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

Session Chair: **KORANA BURKE**

9:00 am – 9:40 am: Fluctuation theorem for Relativistic Brownian motion with Non-Markovian Continuous and Discrete Feedback Control

Priyo Shankar Pal
UMBC

Fluctuation theorems are exact relations that express universal properties of probability distribution of thermodynamic quantities. To elucidate the effect of special relativity on non-equilibrium thermodynamics, this work analyzes fluctuation theorems in relativistic Brownian motion under both, continuous and discrete feedback. An important insight of our work is that information takes a finite time to reach from one point in space-time to another, thereby making the feedback mechanism non-Markovian. As main results, we discuss new fluctuation theorems for such relativistic processes far from equilibrium, which are illustrated for some examples.

Joint work with Sebastian Deffner

9:40 am – 10:20 am: Tailoring stochastic thermodynamics for Bose-Einstein condensates

Frederico Brito
University of Saõ Paulo, Saõ Carlos

The physics of out-of-equilibrium small scale systems emerges as one of the protagonists of contemporary science, mainly due to the advent of quantum technologies and the improvement of means for assessing biological engines. By the application of fluctuation theorems and stochastic thermodynamics, essential progress has been made in this arena, not only providing meaningful connections between thermodynamics and (quantum) information as well as leading to what is known as quantum fluctuation theorems. Due to its practical facet, it is about time to put forward suitable approaches for experimental implementations, with clear means for identifying the measured data and stochastic quantities. In this talk, it is presented an approach developed for Bose-Einstein condensates, where the stochastic entropy production can be directly measured. Such a result broadens the scope of stochastic thermodynamics for more complex quantum systems.

Joint work with Sérgio Muniz and Sebastian Deffner.

10:20 am – 11:00 am: Coffee break

11:00 am – 12:20 am: Tutorial for graduate students and postdocs: Presenting

12:20 pm – 01:00 pm: Lunch

06:00 pm – 09:00 pm: TSRC barbecue at the Tent behind Telluride Intermediate School

2.9 Thursday, August 01, 2019: Thermodynamics of information

8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

Session Chair: **SEBASTIAN DEFFNER**

9:00 am – 9:40 am: Uncertainty tradeoffs in biochemical information processors

Zhiyue Lu
University of North Carolina at Chapel Hill

Living systems respond to external stimuli by utilizing compartmentalized chemical reactions that functions as cellular information processors. A salient example is the single-cell circadian clock (i.e. the Kai-ABC oscillator in cyanobacteria). Such circadian clocks process external signal (sunlight intensity) and computes the time during the day/night. These microscopic "computers" are naturally challenged by two main sources of uncertainty - the internal thermal fluctuations and the external noisy signal. To optimize their performance, we find that a clock must make a tradeoff between resisting internal thermal fluctuations and external signal noise. This noise tradeoff relation reveals the optimal design of a clock given the intensity of two types of noise. Experimental discovery of distinct circadian clocks in two species of cyanobacteria supports our theoretical prediction.

9:40 am – 10:20 am: A realization of an information machine with correlated measurements

Saar Rahav
Technion

The connection between information and thermodynamics has been fascinating scientists ever since Maxwell envisioned his celebrated demon. Technological progress now allows realizing in the lab this celebrated idea, that was originally conceived as a thought experiment. Indeed, recent years have seen experimental realizations of several types of information engines.

In this talk, I will describe a realization of Maxwell's demon in which a colloidal particle is "directed" against a fluid flow. Beyond its appealing simplicity, our experimental setup also exhibits an almost full conversion of information to useful work, since it allows to control how much work is applied directly on the particle. Another feature of the setup is a frequent repeated measurement of the particle location, resulting in nontrivial correlations between the outcomes of consecutive measurements. The effect of these correlations on the useful information acquired is investigated with the help of computer simulations.

1. T. Admon, S. Rahav, and Y. Roichman, "Experimental Realization of an Information Machine with Tunable Temporal Correlations", Phys. Rev. Lett. **121**, 180601 (2018)

10:20 am – 11:00 am: Coffee break

11:00 am – 12:20 pm: Tutorial for graduate students and postdocs: Proposal writing

12:20 pm – 01:00 pm: Lunch

2.10 Friday, August 02, 2019: Thermodynamic control II

8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

Session Chair: **KORANA BURKE**

9:00 am – 9:40 am: Energy absorption in classical periodically driven chaotic systems

Wade Hodson
University of Maryland, College Park

Developing techniques to limit energy absorption, or "heating", is essential for stabilizing interesting states of driven systems. Motivated by recent work on quantum time crystals and related phenomena, we explore the mechanisms that lead to heating in classical chaotic systems subject to periodic driving. Our investigation proceeds primarily in the context of an "energy diffusion" model, in which the energy distribution of a driven system is seen to evolve according to a Fokker-Planck equation. We discuss some properties of this model, and compare it to other approaches, with a particular focus on the limit of high-frequency driving, where high-frequency perturbative methods can be invoked. We conclude with some discussion of how results for this classical system may provide insight into the heating of analogous quantum systems.

9:40 am – 10:20 am: Controlling protein dynamics through counterdiabatic driving

Michael Hinczewski
Case Western Reserve University

Shortcuts to adiabaticity provide powerful tools for the control of quantum systems, allowing adiabatic evolution over finite time intervals. These methods also have direct mathematical analogues in classical stochastic systems. In particular, one can maintain the instantaneous equilibrium distribution of a Markovian system with time-varying transition rates by adding additional "counterdiabatic" corrections to the rates. In this talk, we will explore the implementation of these ideas in the context of protein folding biophysics. We consider two examples, one in vivo and the other in vitro. The first example concerns so-called molecular chaperones: these are protein enzymes that facilitate the unfolding or disaggregating of misfolded proteins. Such chaperones constitute an elaborate, continuously operating machinery within the cell, since many newly synthesized proteins are susceptible to misfolding. Environmental stresses exacerbate the problem: temperature increases by just a few degrees can significantly enhance the tendency of proteins to misfold, and the cell responds by rapidly upregulating chaperone concentration—part of process known as heat shock response. Since chaperone operation typically requires a constant energy input in the form of ATP hydrolysis, the probability distribution of conformational states for the proteins which the chaperones control is generally out of thermal equilibrium. Thus nonequilibrium driving is an essential aspect of the heat shock response. We show how the cell can harness counterdiabatic strategies to minimize time lag and move efficiently from one nonequilibrium distribution to another over finite time intervals. In the second example, we analyze force spectroscopy experiments, where the stability of folded protein states is studied by using an atomic force microscope to rapidly increase the force on single protein molecules. Because adiabatically slow pulling may be hard to realize in practice, various nonequilibrium artifacts often cloud the interpretation of the experimental results. We show how a counterdiabatic protocol allows the experimentalist to mimic the adiabatic case while pulling at an arbitrarily fast rate. This eliminates the artifacts, yielding better estimates of intrinsic protein properties from the experimental data.

10:20 am – 11:00 am: Coffee break

11:00 am – 11:40 am: Thermodynamics of Unsupervised Learning from Small Data: Autonomous One-Shot Work Production as a Performance Measure

Alec Boyd
Nanyang Technological University

Thermodynamic agents are able to use information in their environment as a thermodynamic resource to produce work. This is reflected in Landauer's Principle, which bounds the average work production by the change in state-space entropy. However, what if an agent's input is characterized finite data, rather than a distribution over inputs? We derive an expression for the agent's work production for particular computational trajectories (input-output pairs), as opposed to the work production averaged over all possible inputs and outputs. Here we consider an agent that receives a time series of inputs from its environment, transducing the inputs into outputs to perform a computation. We calculate the work production when the computation operates on a particular finite time series. While this expression is difficult to calculate for agents performing arbitrary

computations, if the agent is designed to produce the most work from an anticipated input sequence distribution, the work production simplifies to an expression which is dominated by the log-likelihood of the input sequence given the anticipated input sequence distribution. Thus, we arrive at a striking connection to unsupervised machine learning, for which the log-likelihood is a common performance measure of the effectiveness of the anticipated distribution as a model of the process that generated the data. With this connection, we treat the input sequence as training data and the work production as a performance measure. We evaluate the average dissipated work from new inputs given that the actual input distribution doesn't match the anticipated distribution. Again, we see a connection to unsupervised machine learning, as the dissipated work is proportional to the model-dependent term in the expected risk. However, if the agent is designed to harness maximal work from its training data, with arbitrary memory, then the agent overfits. This leads to unnecessarily complex agents for small training time-series. And we see dire energetic consequences to overfitting, as it is highly likely that the optimized agent will dissipate infinitely when applied to new inputs. Thus, we propose a refined class of agents, which are not thermodynamically efficient, but asymptotically harness maximal work from their anticipated input. By less greedily harnessing energy from their training data, we see that these agents only asymptotically approach complex models as the amount of training data merits. Moreover, because these regularized agents adapt more gradually to their input data, they dissipate finite work and entropy for input distributions that don't match their model. Thus, we demonstrate a connection between thermodynamic agents and unsupervised machine learning, which leads to physically motivated modifications to machine learning performance measures that avoid overfitting to training data.

11:40 am – 12:20 pm: Closing Remarks

James P. Crutchfield
Korana Burke
Sebastian Deffner

3 Conference Venue and Maps

Conference will be held at:
Telluride Intermediate School, 725 W Colorado Ave Telluride, CO 81435

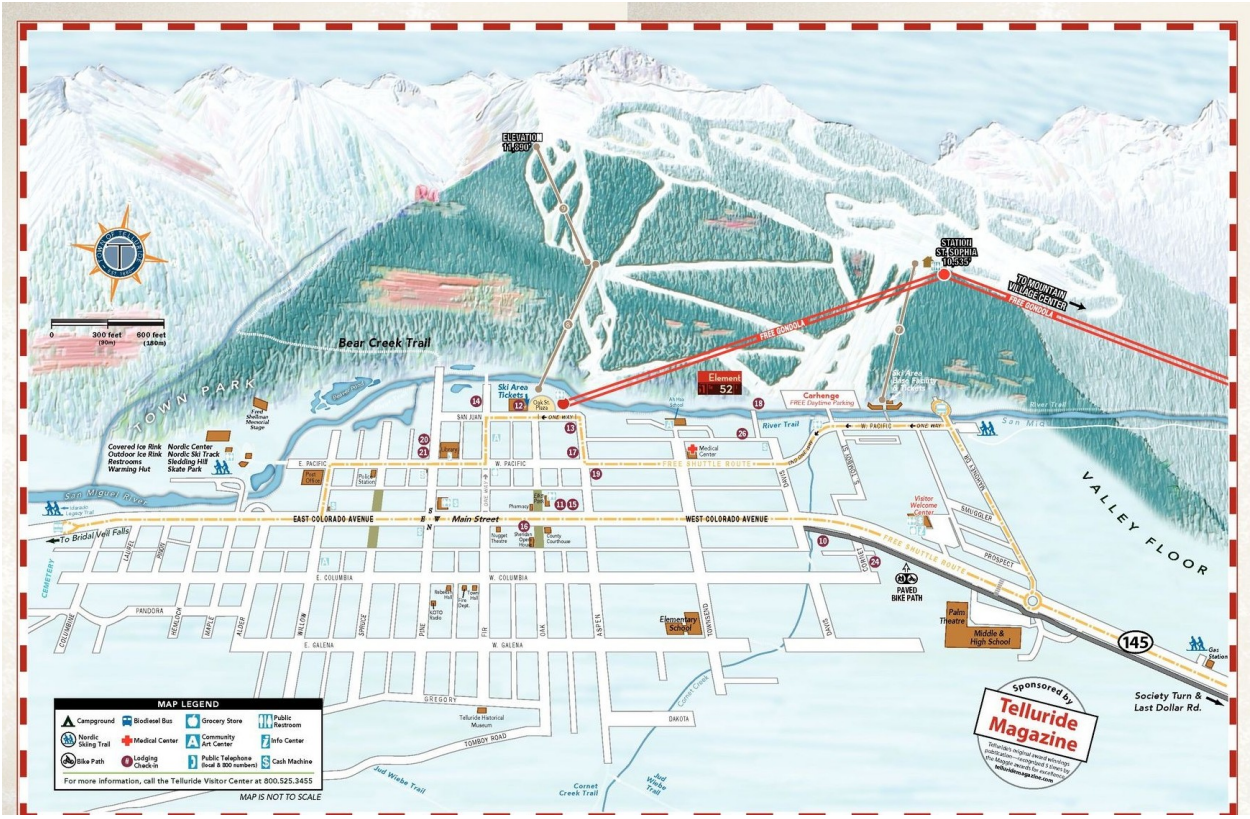

Figure 3.1: Map of the Town of Telluride

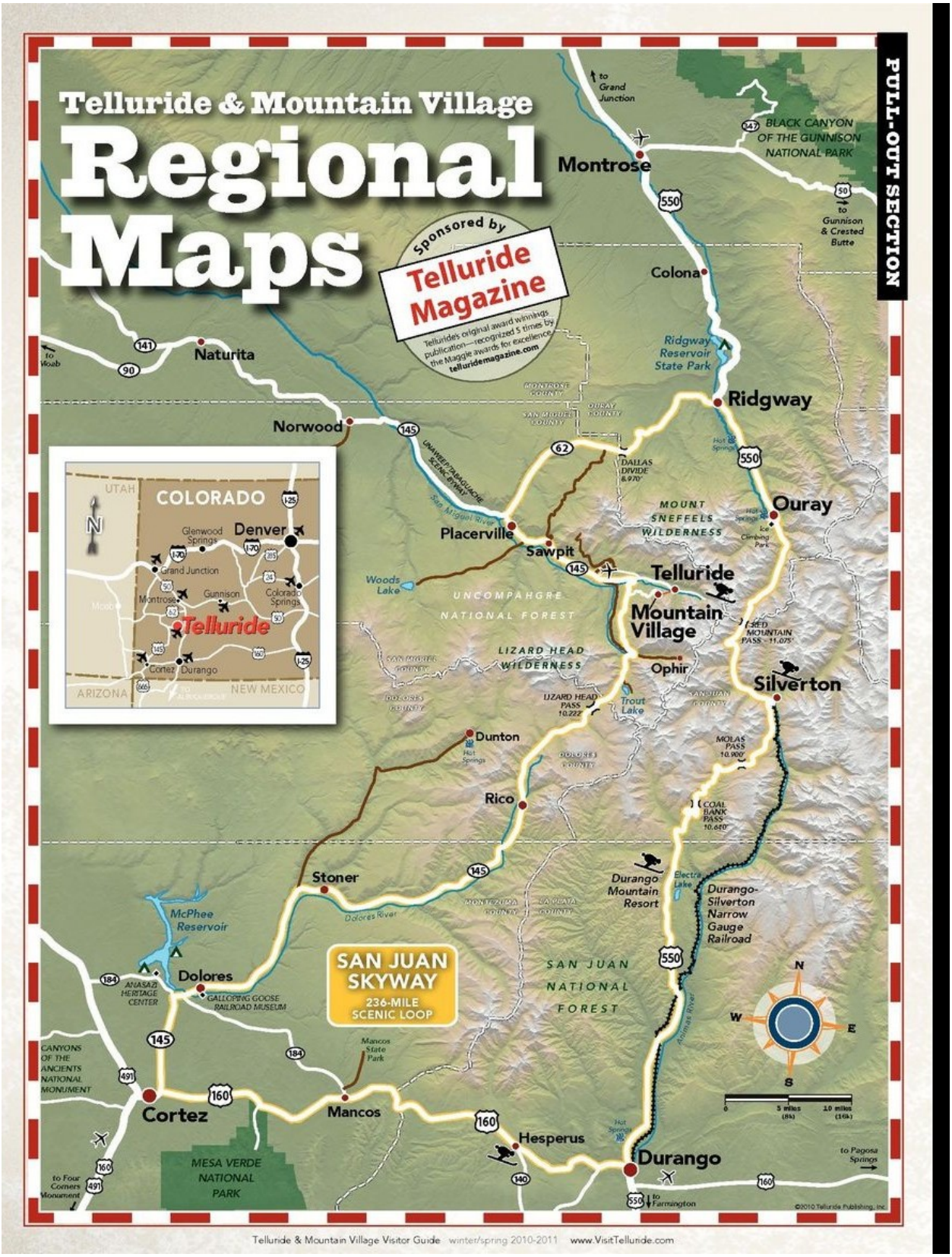

Figure 3.2: Regional Map

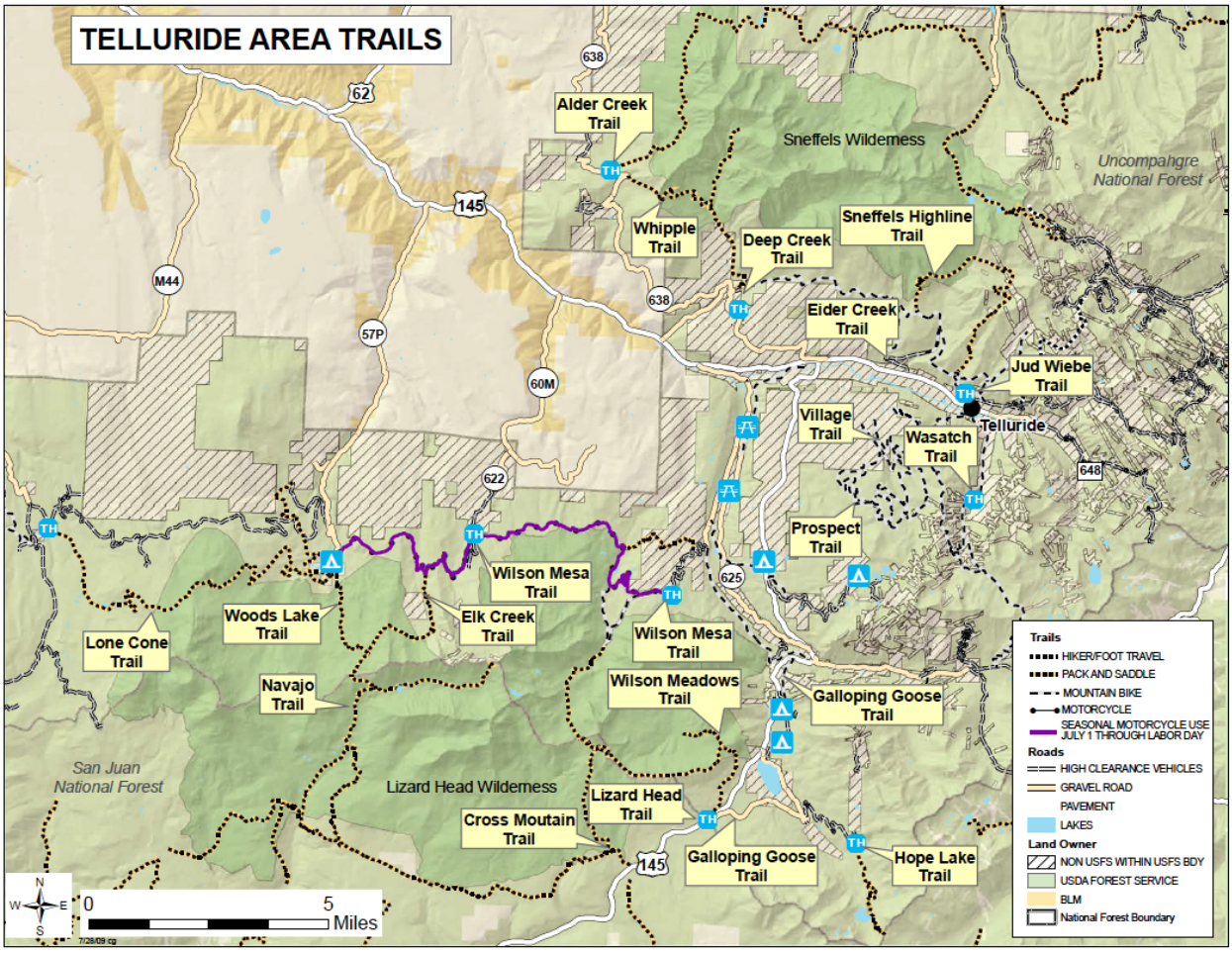

Figure 3.3: Telluride Area Trail Map