

# Information Engines at the Frontiers of Nanoscale Thermodynamics

## Organizing Committee:

Fabio Anza James Crutchfield Korana Burke Sebastian Deffner

July 20 - July 29, 2022

Telluride Intermediate School, 725W Colorado Ave<br/> Telluride, CO81435

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# 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.

• On Wednesday, July 27, 2022 we are going to have a joint session with the workshop *Optimizing Thermodynamic Systems* organized by our friends Peter Salamon and Karl Heinz Hoffmann. The session will take place in the Depot.

## 2.2 COVID-19 Guidlines

We are committed to making this workshop safe and enjoyable for all participants. We wish to be a vaccinated community. Please bring proof of vaccination (including all boosters available in your local community). Due to increasing cases and the presence of highly contagious COVID-19 variants, we request that all participants get tested when they arrive and retest three days later. We acquired two antigen tests for each participant. You can pick these up at check in. We also request that all participants wear masks whenever possible. We will have masks available for our workshop in case you forget yours. If anyone tests positive and so misses the workshop, we will have ways for you to participate remotely.

Friday 07/29	breakfast	$\operatorname{Boyd}$	Hinczewski	coffee	$\operatorname{Rupe}$	$\operatorname{Ray}$	lunch										
Thursday 07/28	breakfast	DeWeese	Frim	coffee	Zhong	Wimsatt	lunch										
Wednesday $07/27$	breakfast	Deffner		coffee	Round table	Round table	lunch	Joint session			TSRC bbq	TSRC bbq	TSRC bbq				
$\begin{array}{c} {\rm Tuesday} \\ 07/26 \end{array}$	breakfast	$\mathbf{Green}$	$\mathbf{Aifer}$	coffee	workshop	workshop	lunch								town talk		
Monday 07/25	breakfast	Habermehl	Scherer	coffee	Chamberlin	Semaan	lunch								Group dinner	Group dinner	Group dinner
$\left\  \begin{array}{c} \text{Sunday} \\ 07/24 \end{array} \right $																	
Saturday 07/23	breakfast	Jurgens	Gier	coffee	Venegas-Li	$\mathbf{Riechers}$	lunch										
Friday $07/22$	breakfast	$\mathbf{Z}$ wolak	Anza	coffee	Majidy	$\mathbf{Lasek}$	lunch								Pizza party	Pizza party	Pizza party
$ m Thursday \ 07/21$	breakfast	opening	Crutchfield	coffee	${f Jarzynski}$	$\mathbf{L}\mathbf{u}$	lunch										
Wednesday $07/20$	breakfast	meet $\&$ greet	meet & greet	coffee	meet & greet	meet $\&$ greet	lunch										
	8:20	9:00	9:40	10:20	11:00	11:40	12:20	13:00	13:40	14:20	15:00	15:40	16:20	17:00	17:40	18:20	19:00

## 2.3 Wednesday July 20, 2022: Meet & Greet

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

Check-In and breakfast at the Telluride Intermediate School

### 9:00 am - 10:20 am: Introductions

Fabio Anza James P. Crutchfield Korana Burke Sebastian Deffner

10:20 am - 11:00 am: Coffee break

11:00 am - 12:20 am: Round table and free discussions

Fabio Anza James P. Crutchfield Korana Burke Sebastian Deffner

12:20 pm - 1:00 pm: Lunch

### 2.4 Thursday, July 21, 2022: Maxwellian demons

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

Check-In and breakfast at the Telluride Intermediate School

Session Chair: FABIO ANZA

### 9:00 am - 9:40 am: Opening talk

Fabio Anza James P. Crutchfield Korana Burke Sebastian Deffner

### 9:40 am – 10:20 am: Demonology: The Curious Role of Intelligence in Physics & Biology

James P. Crutchfield University of California Davis

For the lion's share of its history, physics analyzed the inanimate world. Or, that is the view it has of itself. Careful reflection, though, shows that physics regularly invoked an expressly extraphysical agency – intelligence – in its efforts to understand even the most basic physical phenomena. I will survey this curious proclivity, noting that similar appeals to intelligent "demons" go back to Laplace's theory of chance, Poincaré's discovery of deterministic chaos in the solar system, and Darwin's explanation of the origin of biological organisms in terms of natural selection. Today, we are on the verge of a new physics of information that is transforming problematic "demonology? to a constructive, even an engineering, paradigm that explains information processing embedded in the natural world. To illustrate I will show how deterministic chaos arises in the operation of Maxwell's Demon and outline nanoscale experimental implementations ongoing at Caltech's Kavli Nanoscience Institute.

### 10:20 am - 11:00 am: Coffee break

# 11:00 am – 11:40 am: From non-autonomous feedback control to autonomous information ratchet

### Christopher Jarzynski

University of Maryland, College Park

I will discuss a simple strategy for converting a non-autonomous Maxwell demon, driven by feedback control operated by an external agent, into an autonomous information ratchet, which operates by writing information to a memory register. The strategy makes use of the underlying network structure of the non-autonomous model to design appropriate bit interaction rules for the autonomous model. The strategy will be illustrated on a model of a feedback-controlled double quantum dot, recently introduced by Annby-Andersson et al (Phys Rev B, 101, 165404, 2020). The corresponding autonomous model can be solved analytically in the limit of long bit-system interaction times, and for finite interaction times semi-analytical phase diagrams of operational modes are obtained and compared with stochastic simulations. This work was performed in collaboration with Debankur Bhattacharyya.

# 11:40 am – 12:20 pm: Can simple bio-signaling receptors simultaneously report multiple environmental information?

### Zhiyue Lu

University of North Carolina at Chapel Hill

Yes! Biological sensory receptors provide perfect examples of microscopic scale information transduction in the presence of thermal fluctuations. For example, studies of ligand-receptor interactions show that accurate concentration sensing is achieved by integrating noise in the sensor's stochastic trajectories. We argue that the stochastic trajectory is not always an adversary. Instead, it could allow multiplexing by a single sensor via simultaneous transduction of multiple environmental variables (e.g., concentration, temperature, and flow speed) to the downstream sensory network. We develop a general theory of stochastic sensory multiplexing for bio-sensory receptors and suggest a theoretical upper bound. The theory is demonstrated and verified by an exactly solvable Markov model, where an arbitrary sensor achieves the upper bound without optimization. The theory is further demonstrated by a realistic Langevin dynamics simulation of a ligand-receptor sensor in a bath of ligands. Simulations verify that even a binary-state ligand receptor with short-term memory can simultaneously sense two out of three (ligand concentration, temperature, and media's flow speed) independent variables. Both models demonstrate that the upper bound for multiplexing is tight. This theory also provides insights into the design of novel microscopic sensors capable of multiplexing in complex environments

### 12:20 pm - 1:00 pm: Lunch

## 2.5 Friday, July 22, 2022: Quantum information and thermodynamics

### 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: A resource theory for quantum observers of the classical

### Michael Zwolak

National Institute of Standards and Technology

We live in a quantum Universe, and quantum systems change their state when observed; they are re-prepared by measurements. Observers – from humans down to microscopic organisms – have to learn, respond, and adapt within this unpredictable medium. In our world, observers acquire information about quantum systems indirectly via redundantly encoded information in the environment. Here, we demonstrate that redundancy confers stability and robustness to observation. Provided a guarantee– a "promise" by Nature – of (approximately) homogeneous environment states and interactions, a single optimal measurement emerges independently of the system's state. Only the environment's entropy modifies this optimum, but only after an abrupt transition as the entropy approaches zero. Moreover, a quantum memory does not impart a substantial advantage when acquiring redundant information. Even modest measurement capabilities can efficiently access redundant information. These results suggest a paradigm where nascent life can begin with nearly any observational resources (robustness) and evolve towards a fixed optimum (stability).

# 9:40 am – 10:20 am: Geometric tools for the phenomenology of out-of-equilibrium quantum systems

### Fabio Anza

University of Washington

In the past 30 years, quantum information processing technologies have moved from a purely theoretical effort to a disruptive technology with the potential to impact society at the larger scale. The efforts to scale up these technologies are currently bringing in new and unexpected challenges. These require new concepts and techniques to understand, model, control, and predict the behavior of quantum systems. Geometric quantum mechanics is a differential-geometric approach to quantum mechanics that provides new tools of analysis to help in the forthcoming challenges of modeling complex quantum systems and leveraging their information processing capabilities. In the past 3 years, in collaboration with J. Crutchfield, S. Deffner and other researchers, I have developed a plethora of geometric tools to improve our understanding of complex (out-of-equilibrium and many-body) quantum systems. In this talk, I will report on the most recent results, ongoing efforts and future challenges

### 10:20 am - 11:00 am: Coffee break

### 11:00 am – 10:40 am: Noncommuting charges: Bridging theory to experiment

### Shayan Majidy

Institute for Quantum Computing

Noncommuting conserved quantities have recently launched a subfield of quantum thermodynamics. In conventional thermodynamics, a system of interest and an environment exchange quantities – energy, particles, electric charge, etc.– that are globally conserved and are represented by Hermitian operators. These operators were implicitly assumed to commute with each other, until a few years ago. Freeing the operators to fail to commute has enabled many theoretical discoveries – about reference frames, entropy production, resource-theory models, etc. Little work has bridged these results from abstract theory to experimental reality. This work provides a methodology for building this bridge systematically: we present a prescription for constructing Hamiltonians that conserve noncommuting quantities globally while transporting the quantities locally. The Hamiltonians can couple arbitrarily many subsystems together and can be integrable or nonintegrable. Our Hamiltonians may be realized physically with superconducting qudits, with ultracold atoms, and with trapped ions

# 11:40 am – 12:20 pm: Experimental observation of thermalisation with noncommuting charges

### Aleksander Lasek

University of Maryland, College Park

Quantum simulators have recently enabled experimental observations of quantum many-body systems' internal thermalisation. Often, the global energy and particle number are conserved, and the system is prepared with a well-defined particle number – in a microcanonical subspace. However, quantum evolution can also conserve quantities, or charges, that fail to commute with each other. Noncommuting charges have recently emerged as a subfield at the intersection of quantum thermodynamics and quantum information. We initiate the experimental testing of its predictions, with a trapped-ion simulator. We prepare 6-15 spins in an approximate microcanonical subspace, a generalisation of the microcanonical subspace for accommodating noncommuting charges, which cannot necessarily have well-defined nontrivial values simultaneously. The noncommuting charges are the three spin components. We simulate a Heisenberg evolution using laser-induced entangling interactions and collective spin rotations. We report the first experimental observation of a novel non-Abelian thermal state, predicted by quantum thermodynamics. We observe reduced manybody thermalization in the presence of noncommuting charges. Quantum non-commutation effects are detectable and significant for relatively large realistic systems, despite decoherence. This work initiates the experimental testing of a subfield that has so far remained theoretical.

### 12:20 pm - 1:00 pm: Lunch

### 6:00 pm - open end: Pizza party

### 2.6 Saturday, July 23, 2022: Stochastic processes

### 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: Ambiguity Rate of Hidden Markov Processes

### Alexandra Jurgens

University of California Davis

The epsilon machine is a stochastic process' optimal model—maximally predictive and minimal in size. It often happens that to optimally predict even simply-defined processes, probabilistic models—including the epsilon machine—must employ an uncountably-infinite set of features. To constructively work with these infinite sets we have mapped the epsilon machine to a placedependent iterated function system (IFS)—a stochastic dynamical system. This allows us to introduce the ambiguity rate that, in conjunction with a process' Shannon entropy rate, determines the rate at which this set of predictive features must grow to maintain maximal predictive power over increasing horizons. The ambiguity rate is also the correction to the Lyapunov dimension of an IFS's attracting invariant set, allowing us to calculate their statistical complexity dimension—the information dimension of the minimal set of predictive features. This result allows us to calculate the statistical complexity dimension for hidden Markov processes in general, which has already found use in the study of the thermodynamics of information processing.

### 9:40 am – 10:20 am: Information Processing with Quantum State Stochastic Processes

#### David Gier

University of California Davis

A quantum information source with memory emits a quantum-state stochastic process (QSSP) consisting of states (e.g., one qubit per timestep) that can be classically-correlated or entangled. We characterize these sequences by their von Neumann entropy rate, quantum excess entropy, and quantum Markov order. These also serve as bounds on the classical properties of measurement outcomes when the quantum states are measured sequentially. By treating these correlated states as information reservoirs we find the entropic cost for a finite-state agent to perform two information processing tasks: synchronizing to a known quantum source and erasing a QSSP. Performance on both tasks is improved when the agent (1) has an accurate predictive model of the source and (2) follows an adaptive measurement protocol rather than measuring each state with the same POVM

### 10:20 am - 11:00 am: Coffee break

### 11:00 am - 11:40 pm: Optimality and Complexity in Quantum-State Stochastic Processes

### Ariadna Venegas-Li

University of California Davis

Temporal sequences of quantum states, when measured by a classical observer, generically result in highly complex classical stochastic processes. The high complexity manifests in two specific ways: (i) the classical process is inherently unpredictable to varying degrees that depend on measurement choice and (ii) their optimal prediction requires using an infinite number of temporal features. We identify the mechanism underlying this complexity as generator nonunifilarity, and discuss the methodology to quantify both the stochasticity and structure of the resulting processes. Making use of these quantifications, we explore the influence of the choice of measurement on the resulting classical process, and propose a set of definitions of measurement optimality.

### 11:40 am – 12:20 pm: Quantum-information engines

### Paul Riechers

Nanyang Technological University

Quantum information-processing techniques enable work extraction from a system's inherently quantum features, in addition to the classical free energy it contains. Meanwhile, the science of computational mechanics affords tools for the predictive modeling of non-Markovian classical and quantum stochastic processes. We combine tools from these two sciences to develop a technique for predictive work extraction from non-Markovian stochastic processes with non-orthogonal quantum outputs. We demonstrate that this technique can extract more work than non-predictive quantum work extraction protocols, on one hand, and predictive work extraction without quantum information processing, on the other. We discover a phase transition in the efficacy of knowledge for work extraction from quantum processes, which is without classical precedent. Our work opens up the prospect of machines that harness environmental free energy in an essentially quantum, essentially time-varying form.

### 12:20 pm - 1:00 pm: Lunch

## 2.7 Sunday, July 24, 2022: Free day

No program, no breakfast or lunch.

## 2.8 Monday, July 25, 2022: Complex Systems and Fluctuations

### 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: Complex Dynamics and Learning in NEMS Oscillator Networks

### Scott Habermehl

California Institute of Technology

Networks of coupled nonlinear oscillators exhibit complex spatiotemporal dynamics which are fundamental to the operation of numerous natural and engineered systems, ranging from the human brain to the North American power grid. However, current laboratory experiments for studying these systems lack the necessary rigor for a deep exploration of the parameter space and, thus, have only examined a tiny slice. Our group is currently building an experimental network of 8 nonlinear oscillators with highly controllable nodes (oscillators) and edges (couplings). This talk will briefly review the underlying technology, nano-electro-mechanical systems (NEMS), and it's nanoscale physics. Then, I will demonstrate how we will use the network as a test platform for exploring nonlinear, high-dimensional, and far from equilibrium systems. Finally, the talk will conclude with a discussion of how the network could be used as a physical reservoir computer, and numerical results exemplifying the predictive capability of the network in different dynamical regimes will be shown. From this work, we can start to understand how networks are able to learn from an input process and what makes a good reservoir for specific tasks.

# 9:40 am – 10:20 am: Optical Matter, Collective Modes, Non-Conservative Forces and Power Dissipation in OM Machines

## Norbert F. Scherer

University of Chicago

Optical Matter (OM) systems - (nano-)particle constituents electrodynamically bound by electromagnetic fields - self-organize into regular but dynamic structures in (focused) optical beams of light. Since OM structures are mechanically overdamped in solution and manifest non-conservative forces due to the continuous power flux, a new perspective is required to describe their collective mechanical modes. We have established that structural changes and reaction coordinates can be expressed in a fluctuation amplitude-based mode basis. Moreover, the power dissipation is modedependent and strong non-conservative forces arise depending on the symmetry of the collective modes and their projection into far-field scattering modes of the electrodynamic field. These effects have consequences for the efficiency of OM machines.

### 10:20 am - 11:00 am: Coffee break

# 11:00 am – 11:40 am: Thermal Fluctuations in Equilibrium: Applications to 1/f noise and information entropy

### Ralph V. Chamberlin

Arizona State University

Equilibrium thermal fluctuations found in many substances exhibit two distinct types of noise as a function of frequency: Johnson-Nyquist (white) noise below about 10 GHz, with excess (1/flike) noise below about 10 Hz. We find that a single model can explain both types of behavior. We start with the standard Ising model and add two crucial features: orthogonal dynamics that separates conservation of energy from conservation of angular momentum (spin alignment), and we treat the transfer of information entropy between the system and its bath explicitly. Simulations of the model on systems of different size show that the maximum 1/f noise occurs in systems of intermediate size. We utilize small-system thermodynamics (nanothermodynamics) as a guide to find systems of optimal size that minimize the 1/f noise

### 11:40 am – 12:20 am: Fluctuations Beyond Detailed Balance in Voltage-Gated Ion Channels

### Mikhael Semaan University of California Davis

Systems exhibiting nonequilibrium steady states (NESSs) produce heat in functionally distinct forms: excess, that dissipated during relaxation to steady state; and housekeeping, that dissipated to maintain the steady state conditions. Building on and extending previous work, we derive and showcase a trajectory class fluctuation theorem (TCFT) for fully general nonequilibrium systems. As corollaries, we highlight connections to two separate Second Laws: one for excess work—most analogous to its equilibrium steady-state counterpart—and one for housekeeping heat, which is unique to the NESS setting. Each of these Second Laws alone are statistically true but can be violated by individual realizations.

Using the TCFT and taking a textbook model of the sodium ion channel as an example, we then show how under realistic action potential driving both of these Second Laws are often violated even by relatively likely trajectories—and taxonomize the rich biophysical behaviors this implies, to which strictly ensemble-based analyses are blind. The generality of our methods thus gives a prescription for uncovering novel thermodynamic functionality in mesoscopic complex systems

### 12:20 pm - 1:00 pm: Lunch

### 6:00 pm - open end: Group dinner

## 2.9 Tuesday, July 26, 2022: Classical and quantum speed limits

### 8:20 am – 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

### Session Chair: FABIO ANZA

### 9:00 am – 9:40 am: Classical speed limits: from chaotic dynamics to dissipation

### Jason R. Green

University of Massachusetts, Boston

Physical systems powering motion or creating structure in a fixed amount of time dissipate energy and produce entropy. An outstanding challenge is to understand how this tension between dissipation and speed emerges from classical, chaotic dynamics. I will discuss our recent progress in coupling nonlinear dynamics and statistical physics with a classical density matrix theory and how it has led to speed limits for dynamical systems. These bounds directly connect the geometries of phase space and information, constraining the relationship between dissipation and time during transient excursions away from equilibrium.

### 9:40 am - 10:20 am: From quantum speed limits to energy-efficient quantum gates

### Maxwell Aifer UMBC

While recent breakthroughs in quantum computing promise the nascence of the quantum information age, quantum states remain delicate to control. Moreover, the required energy budget for large scale quantum applications has only sparely been considered. Addressing either of these issues necessitates a careful study of the most energetically efficient implementation of elementary quantum operations. In the present analysis, we show that this optimal control problem can be solved within the powerful framework of quantum speed limits. To this end, we derive state-independent lower bounds on the energetic cost, from which we find the universally optimal implementation of unitary quantum gates, for both single and N-qubit operations.

### 10:20 am - 11:00 am: Coffee break

11:00 am – 12:20 am: Career development workshop

12:20 pm – 1:00 pm: Lunch

6:00 pm – 7:00 pm: TSRC town talk – tba Cash bar at 5:30 pm.

# 2.10 Wednesday, July 27, 2022: Joint session with *Optimizing Thermodynamic Systems*

### 8:20 am - 9:00 am: Breakfast at TSRC

Breakfast at the Telluride Intermediate School

### Session Chair: KORANA BURKE

### 9:00 am - 10:00 pm: Thermodynamic control - past, present, & future

### Sebastian Deffner UMBC

Tremendous research efforts have been invested in exploring and designing so-called shortcuts to adiabaticity. These are finite-time processes that produce the same final states that would result from infinitely slow driving. Most of these techniques rely on auxiliary fields and quantum control, which makes them rather costly to implement. I will outline an alternative paradigm for optimal control that has proven powerful in a wide variety of situations ranging from heat engines over chemical reactions to quantum dynamics – thermodynamic control. Focusing on only a few, selected milestones I will try to provide a pedagogical entry point into this powerful and versatile framework.

- 10:00 am 10:30 am: Coffee break
- 9:00 am 10:00 pm: Round table thermodynamic control
- 12:00 pm 01:00 pm: Lunch
- 1:00 pm 4:00 pm: Optimizing Thermodynamic Systems

Peter Salamon and Karl Heinz Hoffmann

6:00 pm – 9:00 pm: TSRC barbecue

## 2.11 Thursday, July 28, 2022: Thermodynamic optimization

### 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: Universality of the thermodynamic metric

Michael DeWeese

University of California, Berkeley

Geometrical approaches to understanding and controlling small out-of-equilibrium systems have proven to be very useful, but a mathematically rigorous foundation for these methods has been lacking. Towards this end, we recently derived a perturbative solution to the Fokker-Planck equation for one-dimensional driven Brownian motion in the overdamped limit enabled by the spectral properties of the corresponding single-particle Schrödinger operator. The perturbation theory is in powers of the inverse characteristic timescale of variation of the fastest varying control parameter. We used the theory to rigorously derive an exact formula for a Riemannian "thermodynamic" metric in the space of control parameters of the system, and we found that up to second-order terms in the perturbation theory, optimal dissipation-minimizing driving protocols minimize the length defined by this metric. Intriguingly, we also showed that a previously proposed metric is calculable from our exact formula with corrections that are exponentially suppressed in a characteristic length scale. Despite the apparent differences between our new metric and the previous one, we have now shown that they are in fact identical under very general conditions for a wide range of physical systems. I will finish by describing some open questions and future research directions, such as uncovering the physical meaning of various symmetries of the metric, and understanding and exploiting the geometrical nature of higher order terms in our expansion.

### 9:40 am – 10:20 am: Geometric bound on efficiency of irreversible thermodynamic cycles

### Adam Frim

University of California, Berkeley

Recently, numerous studies have considered the optimal operation of thermodynamic cycles acting as heat engines with a given profile in thermodynamic space (e.g., P-V space in classical thermodynamics), with a particular focus on the Carnot engine. In this talk, I will discuss our recent results using the lens of thermodynamic geometry to explore the full space of thermodynamic cycles with continuously varying bath temperature in search of optimally shaped cycles acting in the slow-driving regime. By applying classical isoperimetric inequalities, we derive a universal geometric bound on the efficiency of any irreversible thermodynamic cycle and explicitly construct efficient heat engines operating in finite time that nearly saturate this bound for a specific model system. Given the bound, these optimal cycles perform more efficiently than all other thermodynamic cycles operating as heat engines in finite time, including notable cycles, such as those of Carnot, Stirling, and Otto. For example, in comparison to recent experiments, this corresponds to orders of magnitude improvement in the efficiency of engines operating in certain time regimes. Our results suggest novel design principles for future mesoscopic heat engines and are ripe for experimental investigation.

### 10:20 am - 11:00 am: Coffee break and group picture

### 11:00 am – 11:40 am: Limited-control optimal protocols arbitrarily far from equilibrium

### Adrianne Zhong University of California, Berkeley

Optimizing the energy efficiency of finite-time processes is of major interest in the study of nonequilibrium systems. Recent studies have explored finite-time dissipation-minimizing protocols for stochastic thermodynamic systems driven arbitrarily far from equilibrium, when granted full external control to drive the system. However, often times in both simulation and experimental contexts, systems may only be controlled with a limited set of degrees of freedom. Here, we apply ideas from optimal control theory to obtain optimal protocols arbitrarily far from equilibrium for this unexplored limited-control setting. By working with deterministic Fokker-Planck probability distribution time evolution and using the first law of thermodynamics to recast the work-expenditure, we can frame the work-minimizing protocol problem in the standard form of an optimal control theory problem. We demonstrate that finding the exact optimal protocol is equivalent to solving a system of Hamiltonian partial differential equations, which in many cases admit efficiently calculatable numerical solutions. Within this framework, we reproduce analytical results for the optimal control of harmonic potentials, and numerically devise novel optimal protocols for two examples: varying the stiffness of a quartic potential, and linearly biasing a double-well potential. We confirm that these optimal protocols outperform other protocols produced through previous methods, in some cases by a significant amount. We find that for the linearly biased double-well problem, the mean position under the optimal protocol travels at a near-constant velocity, and that surprisingly, for a certain timescale and barrier height regime, the optimal protocol is non-monotonic in time.

### 11:40 am – 12:20 am: The Trajectory Class Fluctuation Theorem

### Greg Wimsatt

University of California Davis

The Trajectory Class Fluctuation Theorem (TCFT) is a new tool for nonequilibrium thermodynamics. It treats the thermodynamics of arbitrary measurable subsets of system trajectories. The TCFT can be seen to span a space of fluctuation theorems from Crooks' detailed fluctuation theorem to Jarzynski's Equality. The TCFT also significantly improves estimates on free energy differences over Jarzynski's Equality by countering the problem of the dominance of rare events. We demonstrate this with a protocol on a double-well system. It also leverages information of trajectory class probabilities to provide stronger entropic or work bounds than the second law

### 12:20 pm – 1:00 pm: Lunch

## 2.12 Friday, July 29, 2022: Statistical physics 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: Thermodynamic Overfitting: Limits on Complexity in Thermodynamic Learning

### Alec Boyd

California Institute of Technology

Recent results show that maximizing work production corresponds to thermodynamic learning, guiding information engines towards predictive epsilon-machine models. There is a direct parallel between the maximum-work principle in thermodynamic learning and the maximum-likelihood principle that guides machine learning. However, we show that recklessly maximizing work leads to overfitting, which has dire energetic consequences. We demonstrate that irreversible entropy production diverges when engines are unconstrained in their pursuit of energetic advantage during training. We see that the danger of divergent dissipation and overfitting persists for ever longer strings of training data as the complexity of the information engine's model increases. Thus, functional thermodynamic learning must include physical mechanisms for regularization, to allow the engine to generalize and harvest energy effectively from new information. As a first cut, we propose a physical mechanism for regularization by imposing a uniform initial distribution over the engine's memory. This yields a marked improvement in the thermodynamic performance of complex information engines with larger memories.

#### 9:40 am – 10:20 am: Machine learning in and out of equilibrium

### Michael Hinczewski

Case Western Reserve University

The algorithms used to train neural networks, like stochastic gradient descent (SGD), have close parallels to natural processes that navigate a high-dimensional parameter space, for example protein folding or evolution. In this talk we describe a Fokker-Planck approach, adapted from statistical physics, that allows us to explore these parallels in a single, unified framework. We focus in particular on the stationary state of the system in the long-time limit. In contrast to its biophysical analogues, conventional SGD leads to a nonequilibrium stationary state exhibiting persistent currents in the space of network parameters. The effective loss landscape that determines the shape of this stationary distribution sensitively depends on training details, for example the choice to minibatch with or without replacement. We also demonstrate that the state satisfies the integral fluctuation theorem, a nonequilibrium generalization of the second law of thermodynamics. Finally, we introduce an alternative "thermalized" SGD procedure, designed to achieve an equilibrium stationary state. Deployed as a secondary training step, after conventional SGD has converged, thermalization is an efficient method to implement Bayesian machine learning, allowing us to estimate the posterior distribution of network predictions.

### 10:20 am - 11:00 am: Coffee break

### 11:00 am – 11:40 am: Nonequilibrium Statistical Mechanics and Continuum Computational Mechanics of Partially-Observed Processes

### Adam Rupe

Los Alamos National Laboratory

A system is partially-observed if the accessible observables are insufficient for determining the full state of the system. Past histories of partial observations induce a natural nonequilibrium Maximum Caliber probability measure over the full, unobserved, system states. Together with Koopman and Perron-Frobenius evolution operators, these Maximum Caliber measures define predictive distributions that give optimal stochastic predictions of future observables conditioned on a past history of observables. A continuum generalization of the familiar optimal stochastic models of Computational Mechanics can then be constructed using predictive equivalence. Wiener projections of past histories of observables provide a direct connection to optimal "deterministic" prediction and the Mori-Zwanzig formalism. In ideal cases, both deterministic and stochastic optimal predictive equivalence relation, and the degrees of freedom of the full system (including unobserved DoF) in the ideal case. Similarly, the Markov dynamic over causal states is identical to the dynamics of the full system. Thus, in ideal cases, the optimal stochastic model converges to the true system and its dynamics.

### 11:40 am – 12:20 pm: Gigahertz Sub-Landauer Momentum Computing

#### Kyle Ray

University of California Davis

We introduce a fast and highly-efficient physically-realizable bit swap. Employing readily available and scalable Josephson junction microtechnology, the design implements the recently introduced paradigm of momentum computing. Its nanosecond speeds and sub-Landauer thermodynamic efficiency arise from dynamically storing memory in momentum degrees of freedom. As such, during the swap, the microstate distribution is never near equilibrium and the memory-state dynamics fall far outside of stochastic thermodynamics that assumes detailed-balanced Markovian dynamics. The device implements a bit-swap operation—a fundamental operation necessary to build reversible universal computing. Physically-calibrated simulations demonstrate that device performance is robust and that momentum computing can support thermodynamically-efficient, high-speed, large-scale general-purpose computing that circumvents Landauer's bound.

### 12:20 pm – 1:00 pm: Lunch

# **3 Conference Venue and Maps**

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

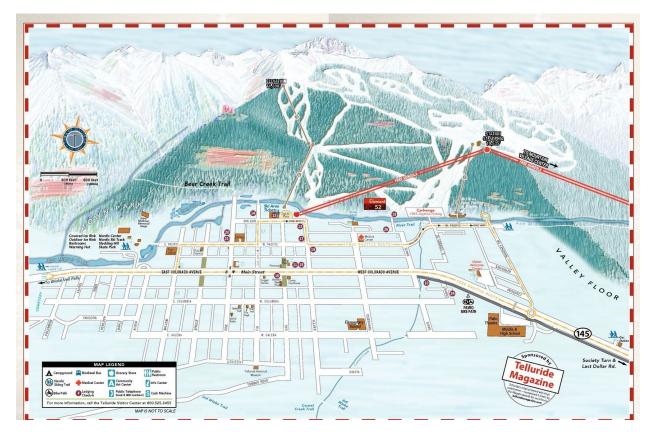


Figure 3.1: Map of the Town of Telluride

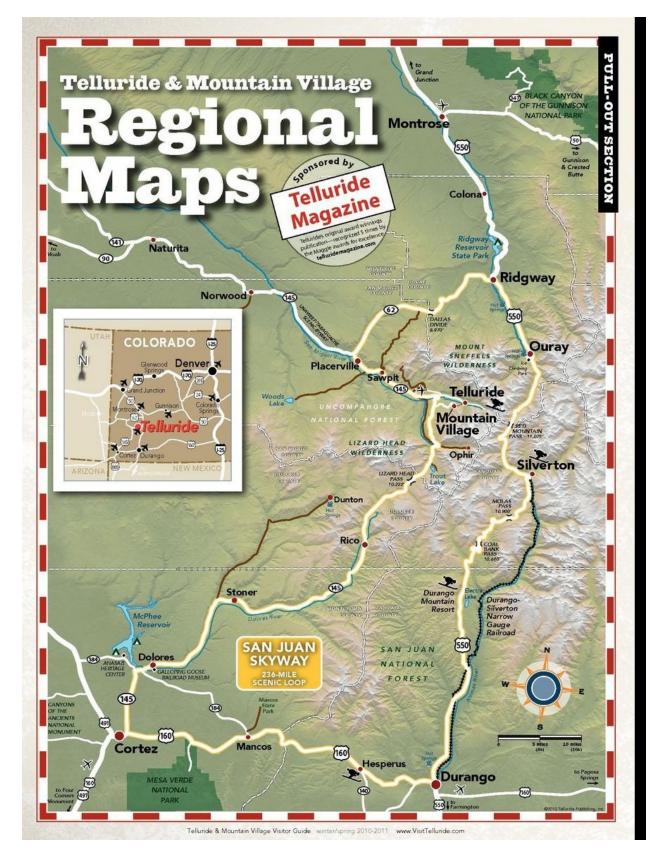


Figure 3.2: Regional Map

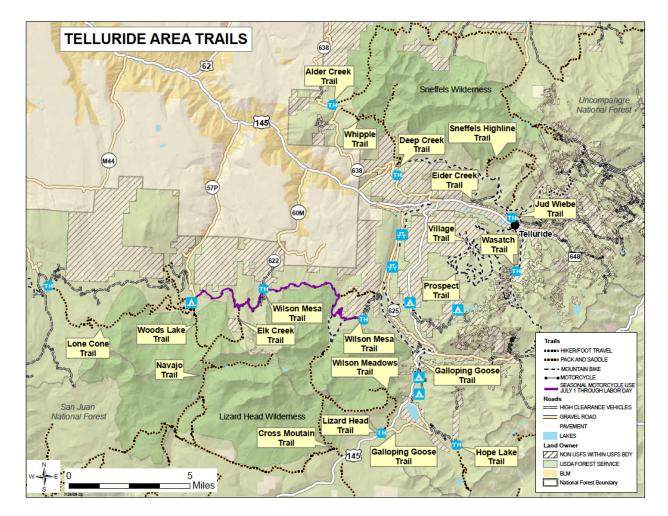


Figure 3.3: Telluride Area Trail Map