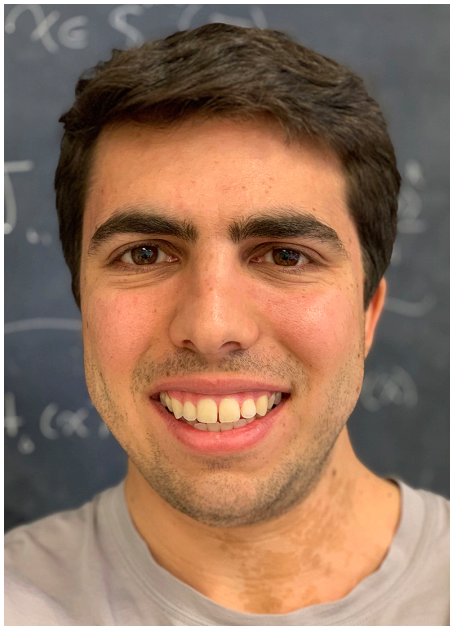
The Adolph C. and Mary Sprague
MILLER INSTITUTE
for Basic Research in Science

Newsletter
Fall 2021

Time evolution of complex systems

Miller Fellow Focus: Reza Gheissari

One of the central goals of modern science is understanding complex systems: these are generally characterized by two hallmarks: large size (many individuals, or variables) and intertwinedness (interactions between these individuals). Fundamental examples of such complexity arise, for instance, in evolutionary biology (a large number of individuals from different species competing over resources), epidemiology (a large population of susceptible, infected, or recovered individuals spreading a virus), protein folding (a large number of amino acids folding into biologically functional conformations), and machine learning (a large number of "neurons" with different activation parameters combining to perform difficult tasks).



All these problems share a central difficulty: the size of the *state space*, or set of possible configurations taken by the variables, grows exponentially with the number of variables. Thus, when the number of variables is on the order of tens, these problems become analytically intractable, and when it is on the order of hundreds, computationally intractable. The field of statistical physics takes a probabilistic perspective to resolve this complexity. Namely, it replaces the uncertainty of individual states in large systems with probability distributions over all their states. One then hopes that macroscopically, the randomness averages out (similar to the classical law of large numbers) in the limit of large system size.

To understand the picture one hopes to obtain from this approach, let us first recall how one would study a *small* system. Consider the example of a single particle performing a state change, say from A to B. The time it takes for the state change to occur grows exponentially as a function of the *activation energy* of the transition A→B. This gives rise to

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Deadline: September 3, 2021

Miller Research Fellowship Nominations
Deadline: September 10, 2021

Miller Research Professorship Applications
Deadline: September 14, 2021

"In summary my time with the Miller institute has been a great experience, giving me a unique opportunity to have a full availability for my research, and in particular plenty of time to read, think, expand my network, exchange ideas, and explore new directions. Thank you so much for supporting my stay in Berkeley. This has been a very precious time for me, but also for my family. I think it will remain as a keystone for building my future research."

Anne Socquet,
Visiting Miller Professor - Spring 2019
University of Grenoble - Alpes

> CONTINUED FROM PAGE 1 [Miller Fellow Focus]

a notion of *metastability*, where a particle is at quasi-equilibrium in one state for a long time before making an unlikely transition to another state, where it quickly equilibrates and remains until the next rare transition. This behavior has been verified mathematically by viewing the particle as performing a *diffusion* (thermally activated random motion) in a bimodal energy potential, where the modes correspond to the states A and B: see **Figure 1.**

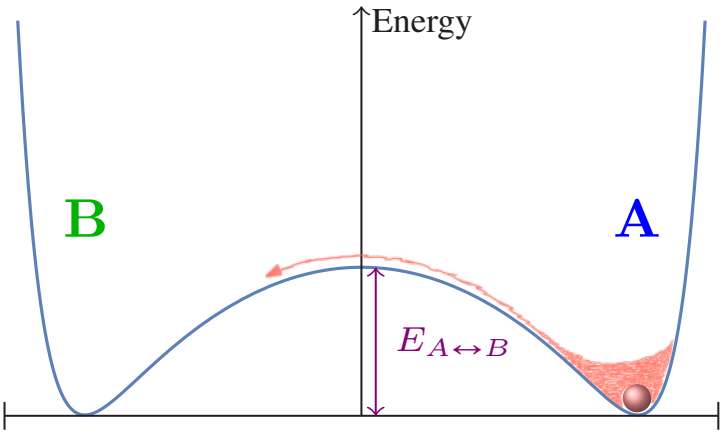


Figure 1. *A particle rests at quasi-equilibrium in state A, then after a time that grows exponentially with the activation energy (purple) transits to state B and equilibrates there.*

A main theme of my research is the development of an analogous mathematical theory for the time evolution of *complex* systems. When moving from a simple system to a complex one, the single particle is replaced by a large number of interacting particles. We call this system "high-dimensional" as there are many variables that must be tracked to determine the current state of the full system.

Let us take as a running example a large number of particles, arranged in some underlying space, each of which may be in state A or B. The reader should feel free to replace the words "state A and B" of "particles" with analogues that are most pertinent to their field: e.g., species labels of individuals in an ecosystem, alleles in a generational tree, or opinions held in a social network. This system becomes complex when the particle states interact with one another. For concreteness, consider an attractive interaction, where particle states, though random, prefer to match their states to those of nearby particles.

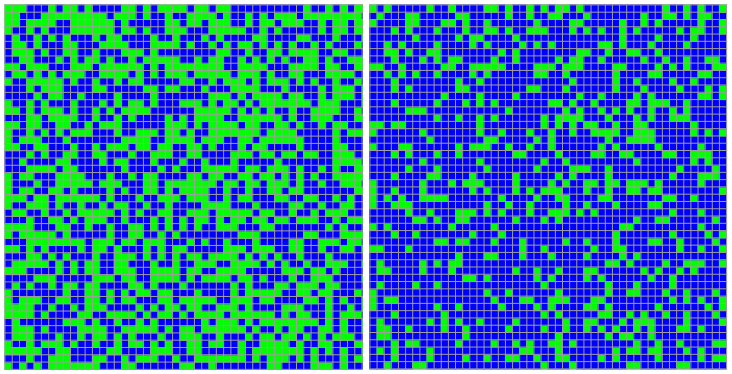


Figure 2. *Configurations in a two-state complex system, consisting of 2500 particles randomly taking states A (blue) or B (green) while wanting to align with their neighbors. On the left, a smaller interaction strength leads to a random-looking configuration, while on the right, a larger interaction strength leads to the system picking one dominant state (in this case, state A).*

This encompasses many two-state complex systems and its equilibrium behavior exhibits a sharp transition as the interaction strength is varied: see **Figure 2**. When the interaction strength exceeds a certain critical value, the interactions dominate the randomness, and the system at equilibrium has two phases, each corresponding to one of the two states A or B being dominant, and the other being subdominant. While the probability distribution over configurations is complicated, one sees this behavior by looking at the distribution only as a function of the *bias*, or number of A particles minus the number of B particles.

More formally, we can consider the *free energy* function of the bias variable. In high-dimensional systems, the free energy is a more relevant quantity than the energy, as it also takes into account the entropy (the number of different configurations having the same bias). The probability distribution gives the largest weight to biases with the smallest free energy. We find that the resulting free energy potential closely resembles the bimodal energy potential of a single particle. See **Figure 3** for a depiction of this analogy.

Consider now the time evolution of this system. Given the analogy of the bias to a single particle system, one might expect that the time evolution of the bias will look like a diffusion in the bimodal free energy potential. In particular, one would expect it to exhibit metastable behavior, spending long periods of time at a quasi-equilibrium in the A-phase (positive bias), before a rare transition to the B-phase (negative bias).

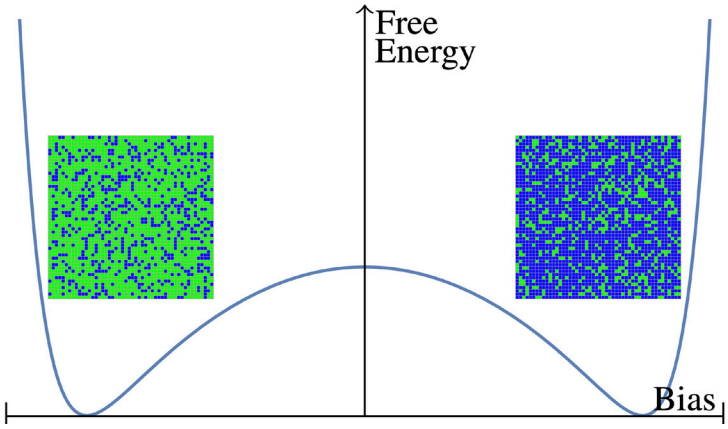


Figure 3. *The free energy, plotted as a function solely of the bias (number of A particles minus number of B particles), gives rise to a bimodal potential similar to that of Figure 1.*

However, this similarity is only heuristic. It is derived by projecting a probability distribution function of a high-dimensional space, onto just a single variable. In particular, the bias in the number of A and B particles cannot distinguish geometric information about locations of the A and B particles. It could be that within the A-phase, there are arrangements, e.g., a solid strip of B's surrounded by A's, which take much longer to equilibrate from than others, e.g., small clusters of B's interspersed among A's. This indicates a subtle difference between the free energy potential of the bias in the complex system and the energy potential of a single particle: here, even inside the A-phase, there are geometrically metastable phases that get lost when only observing the bias.

In recent work as a Miller fellow with Alistair Sinclair, I developed a mathematical foundation to formalize the notion that complex systems quickly reach quasi-equilibrium within a phase. In the context of the above model, we proved that if the system is initialized in "typical" configurations in the A-phase, including in the uniform one (every particles starts in state A), all geometric obstructions to equilibration are in fact avoided. For such initializations, the qualitative system behavior is fully captured by the evolution of the bias, and the predicted metastability picture is valid: the system rapidly reaches a quasi-equilibrium within the A-phase, then waits an exponential time to transition to the B-phase, and so on.

In the 20th century, an extensive mathematical theory of dynamical systems and their diffusion approximations was developed. However, paradigms coming from such systems become more subtle when the dimension of the state space gets large. As ubiquitous as complex systems are, we are only just beginning to develop a mathematically rigorous understanding of their time evolution, including when predictions from their low-dimensional projections are valid, and when they are not. The two-state model described here has presented an important and mathematically tractable testbed for developing such a theory. Extending this theory to richer complex systems with more than two particle types, or non-attractive interactions, is a major focus of my future research.

Reza Gheissari grew up in the suburbs of Los Angeles before moving to Manhattan in 2010 to attend Columbia University, and then to pursue a Ph.D. in mathematics at NYU's Courant Institute. After completing his Ph.D. in 2019, he moved back to California as a Miller Fellow, hosted by Alistair Sinclair and the departments of Statistics and Electrical Engineering and Computer Sciences (EECS). His research is focused on the mathematical foundations of equilibrium and off-equilibrium statistical mechanics, as well as relations to optimization, sampling, and statistical inference in high dimensions. When not thinking about math, Reza enjoys being outdoors, often playing tennis, skiing, and hiking. He is also a member of the Miller Institute's Diversity, Equity, and Inclusion Working Group.

Contact: gheissari@berkeley.edu

Miller Institute weekly lunches resume on campus! With campus starting to return to normal operations, the Miller Institute community is able to gather together each week to connect and share science.

From the Executive Director

Marla Feller, Miller Institute Executive Director & Paul Licht Distinguished Professor in Biological Sciences

If today was not a crooked highway
If tonight was not a crooked trail
If tomorrow wasn't such a long time
Then lonesome would mean nothing to you at all

-Bob Dylan,
Tomorrow is a long time, 1963

Well now THAT was a year! As we come out of this pandemic (fingers crossed!) I have taken some time to reflect on how important human contact is. This lyric from Bob Dylan emphasizes that it takes uncluttered time to create loneliness, which many of us experienced during the height of the pandemic. But through the anxiety, isolation and uncertainty of the past year, the Miller Institute offered a way to connect to one another. The weekly Tuesday zoom lunches and talks and a few (unofficial) in-person, masked events were so key to keeping that sense of community. I want to offer a personal thank you to all of those who participated in these activities.

It is with this spirit of community I am so looking forward to the coming year in the Miller Institute! Starting this year, we have 10 new Fellows, 8 new Miller Professors and 18 Visiting Miller Faculty, including those who postponed their appointments from 2019-2021 as well as the new ones selected for 2021-2022. This year, we welcome UC Berkeley Astronomy Professor Chung-Pei Ma to our Executive Committee and Harvard Evolutionary Biology Professor (and former UC Berkeley Zoology PhD student!) Scott Edwards to our Advisory Board. We welcome back Executive Committee members Professors Roland Burgmann and Yun Song, as well as Advisory Board members Professors Feryal Ozel (University of Arizona), Luis Caffarelli (University of Texas – Austin) and Tim Stearns (Stanford), and we thank them for their continued dedication to the Institute.

The first big event of the year will be our twice-delayed Spring Symposium which will be held this Fall. Many of our speakers from the original planned event in Spring 2020 will be able to attend. We will also be taking advantage of the Fall date to welcome our new Miller Fellows to the event with a daylong retreat before the symposium to help them connect with each other. Stay tuned for photos and stories from the symposium in the next issue. Also this year we will continue our work with a Diversity, Equity, Inclusion and Belonging consultant to interpret the results of the Climate survey and identify improvements. Thank you to all those of you who took time to fill out the survey; your responses will inform our steps to strengthen the Miller Institute.

Summer is also a time we say good-bye to many members of our Miller Community, including 9 of Miller Fellows who will be populating science departments throughout the world while a couple remain at UC Berkeley to continue their research (see Next Steps on p. 6 and the Spring 2021 edition of this newsletter.) And we say goodbye to two of the members of our leadership circle; I want to offer my sincerest appreciation to Professor Steve Leone from Chemistry for his 6 years as a member of our Executive Committee and Professor Steve Block from Biophysics Department at Stanford for his 6 years as a member of our Advisory Committee.

There has also been some change on the Miller Staff last year as the Institute welcomed Vrinda Khanna to join staff members Hilary Jacobsen, Emily Birman and Donata Hubert. Again, I want to acknowledge their hard work and dedication throughout the pandemic; from managing the three competitions, taking care of our current, former and prospective members, and enhancing Miller Institute's online presence, the staff have stayed busy.

We hope you'll stay in touch with us! Follow us on Facebook, Linkedin or Twitter and check our website to read about the many accomplishments of the members of the Miller community as well as links to articles and talks featuring Miller Community Members.

Recent Publications

Kelly Nguyen (Miller Fellow 2016-2019) and **Kathleen Collins** (Miller Professor 2011, Executive Committee Member 2014-2015) are co-authors of the paper, *"Structure of human telomerase holoenzyme with bound telomeric DNA"* published in Nature.

Yu He (Miller Fellow 2019-2020) is a co-author of the article *"Angle-resolved photoemission studies of quantum materials"* published in Rev. Mod. Phys.

Dan Ibarra (Miller Fellow 2019-2021) is a co-author of the paper published by AGU titled *"An Unbroken Record of Climate During the Age of Dinosaurs."*

Soonwon Choi (Miller Fellow 2018-2021) is a co-author of the paper *"Quantum phases of matter on a 256-atom programmable quantum simulator"* published in Nature.

Call For Nominations: Miller Research Competitions

Miller Research Fellowship 2022-2025
Online Nomination Deadline: September 10, 2021

The Miller Institute for Basic Research in Science invites department chairs, faculty advisors, professors and research scientists at institutions around the world to submit online nominations for Miller Research Fellowships in the basic sciences. The Miller Institute seeks to discover and encourage individuals of outstanding talent, and to provide them with the opportunity to pursue their research on the Berkeley campus. The Institute also welcomes nominations for the Kathryn A. Day Postdoctoral Fellowship for outstanding candidates who demonstrate a commitment to outreach in support of science. Fellows are selected on the basis of their academic achievement and the promise of their scientific research. Miller Fellows also have a keen curiosity about all science and share an appreciation for an interdisciplinary experience. The Miller Institute is the sponsor and the administrative home department for each Miller Fellow who is hosted by an academic department. All research is performed in the facilities provided by the host UC Berkeley academic department(s), however remote work may be allowable in accordance with campus policies. A list of current and former Miller Research Fellows is available on our website.

Miller Research Fellowships are intended for exceptional young scientists of great promise who have recently been awarded, or who are about to be awarded, the doctoral degree. Normally, Miller Fellows are expected to begin their Fellowship shortly after being awarded their Ph.D. Applicants who have already completed substantial postdoctoral training are unlikely to be successful except in unusual circumstances. **A nominee cannot hold a paid or unpaid position on the Berkeley campus at the time of nomination or throughout the competition and award cycleaward cycle, which can extend into February**. Nominees who are non-US citizens must be eligible for obtaining J-1 Scholar visa status for the duration of the Miller Fellowship. The Miller Institute does not support H1B visa status. The Fellowship term must commence between July 1 and September 1, 2022. Eligible nominees will be invited by the Institute to apply for the Fellowship. Direct applications and self-nominations are not accepted. *All nominations must be submitted using the Online Nomination System at: **miller.berkeley.edu/fellowship.**

Nominators will need the following required information to complete the online nomination process:
+ Nominee's complete full and legal name (do not use nicknames)
+ Nominee's current institution
+ Nominee's complete, current, and active E-mail address, current mailing address with postal code and telephone number
+ Nominee's Ph.D. Institution and (expected) Date of Ph.D. (month & year required)
+ Letter of recommendation and judgment of nominee's promise by the nominator. Letter must be specific to the Miller Fellowship, have a current date, and be on institutional letterhead. The Executive Committee finds it helpful in the recommendation letter to have the candidate compared with others at a similar stage in their development.
+ Nominator's current active E-mail address, title, and professional mailing address (include zip code/campus mail code.)

The Institute provides a stipend of $68,000 with annual increases on subsequent anniversary dates and an annual research fund of $10,000, for total initial compensation of $78,000. There is provision for travel to Berkeley for Miller Fellows and their immediate families and a maximum allowance of $3,000 for moving personal belongings. Benefits, including medical, dental, vision and life insurance are provided with a modest contribution from the Miller Fellow. All University of California postdocs are represented by the UAW. Fellowships are awarded for three years, generally beginning August 1, 2022 and ending July 31, 2025. Approximately eight to ten Fellowships are awarded each year. Candidates will be notified of the results of the competition starting in mid-December, and a general announcement of the awards will be made in the spring.

Miller Research Professorship AY 2022 - 2023
Online Application Deadline: September 14, 2021

The Miller Professorship program is pleased to announce the call for applications for terms in AY 2022-2023. The objective of the Miller Professorship program is to provide opportunities for UC Berkeley faculty to pursue new research directions on the Berkeley campus and to participate in the vibrant interdisciplinary Miller community. For some, this may best be enabled by taking time off from teaching. For others, the teaching obligations are critical to maintaining campus academic programs. Thus the option for Miller Professors to continue campus service and teaching. Funds will be distributed differently depending upon the choice selected. Details of the terms and the application procedure are posted on the Miller Institute website. The primary purpose of the Miller Professorship program and the evaluation criteria continues to be research excellence. Applicants are encouraged to describe their interest in participating in the Miller Institute community.

Applications from UC Berkeley faculty for Miller Research Professorship terms in the 2022-23 academic year are being accepted online now. Appointees are encouraged to follow promising leads that may develop in the course of their research.

Applications are judged competitively and are due by September 14, 2021. It is anticipated that between five to eight awards will be made. Applications are available at our website: **miller.berkeley.edu/professorship**.

Visiting Miller Research Professorship AY 2022 - 2023
Online Nomination Deadline: September 3, 2021

The Advisory Board of the Miller Institute for Basic Research in Science invites Berkeley faculty to submit online nominations for Visiting Miller Research Professorships and the Gabor A. and Judith K. Somorjai Visiting Miller Professorship Award for terms in Fall 2022 or Spring 2023. The purpose of these Visiting Miller Professorships is to bring promising or eminent scientists to the Berkeley campus on a short-term basis for collaborative research interactions. It is required that awardees be in residence at Berkeley during their appointment term. Faculty members or research scientists from any place in the world are eligible to be considered for sponsorship. Non-US citizens must be eligible for J-1 Scholar visa status. Faculty members at other UC campuses are eligible to be nominated for this program. The Miller Institute, as the sponsor and administrative department, will extend the invitation to the nominee after advising the nominator of its selection. All nominations must be submitted using the Online Nomination System at **miller.berkeley.edu/visiting-professorship**.

Emeritus Miller Institute Members!

Do you wish to receive the Miller Institute newsletter at your home address? Please email millerinstitute@berkeley.edu with your updated address information so as not to miss a single issue.

In the News

(see more past & current Miller Institute News: miller.berkeley.edu/news)

Jeremy Thorner (Miller Professor 1984-1985, 1999-2000) received the prestigious **2022 Centenary Award** from The Biochemical Society *"for his contributions to our understanding of biological signal transduction mechanisms."* The Centenary Award, once called the Jubilee Award, is given annually to a biochemist of distinction from any country.

Bin Yu (Miller Professor 2004, 2016-2017) was awarded an **Honorary Doctorate from the University of Lausanne (UNIL)**, Faculty of Business and Economics, in Switzerland, as *"one of the most influential researchers of her time in Statistics and Data Science, for the excellence and impact of her work, and for her major contributions to the development and advancement of machine learning."*

Miller Members **Prashant Jain** (Miller Fellow 2008-2011), **Mikhail Shapiro** (Miller Fellow 2011-2013) and **Ahmet Yildiz** (Miller Professor 2016-2017) were named finalists of the **2021 Blavatnik National Awards for Young Scientists**, the world's largest unrestricted prize honoring early-career scientists and engineers.

Jacqueline Cherfils (Visiting Miller Professor 2016) was elected a new **member of the European Molecular Biology Organization** in recognition of *"research excellence and the outstanding achievements made by a life scientist."*

Mark Hauber (Miller Fellow 2002-2005) was selected to receive a **Humboldt Research Award** in recognition of his entire academic record in integrative biology to date.

Xie Chen (Miller Fellow 2012-2014) and **L. Mahadevan** (Visiting Miller Professor 2006) were named **2021 Simons Foundation Investigators.**

Miller Members among newly elected **2021 AAAS Fellows:**

- **Odile Eisenstein** (Visiting Miller Professor 2004)
- **Jonas Peters** (Miller Fellow 1998-1999)
- **Ashvin Vishwanath** (Miller Professor 2009)

Michael Jordan (Miller Senior Fellow 2019-Present) and **Sjors Scheres** (Visiting Miller Professor 2015) were among the newly elected **Fellows and Foreign Members of the Royal Society.**

Miller Members among newly elected **2021 NAS Fellows:**

- **Donna Blackmond** (Visiting Miller Professor 2003)
- **Odile Eisenstein** (Visiting Miller Professor 2004)
- **Glenn Fredrickson** (Visiting Miller Professor 1993)
- **N. Louise Glass** (Miller Professor 2011-2012)
- **Ursula Keller** (Visiting Miller Professor 2006)
- **Michael Turelli** (Miller Professor 2006)

The mural "Horizon Light" was inspired by **Chung-Pei Ma's** (Miller Professor 2010, 2019-2020, Executive Committee 2021) research which focuses on supermassive black holes. The mural, located in San Carlos CA, celebrates women of color in STEM.

Miller Members named **2021 John Simon Guggenheim Memorial Foundation Fellows:**

- **William Bialek** (Miller Fellow 1986-1987) for his research in a variety of theoretical problems at the interface of physics and biology, from the dynamics of individual biological molecules to learning and cognition.
- **Christopher Chang** (Miller Professor 2011-2012) for his research on metals in biology and energy. He pursued new concepts in sensing and catalysis that draw from core disciplines of inorganic, organic and biological chemistry.

Manos Mavrikakis (Visiting Miller Professor 2019) was the recipient of the **2021 Robert Burwell Lectureship in Catalysis** *"in recognition of substantial contributions to one or more areas in the field of catalysis with emphasis on discovery and understanding of catalytic phenomena, catalytic reaction mechanisms and identification and description of catalytic sites and species."*

Next Steps

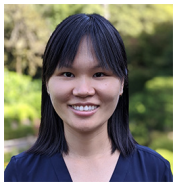
The Miller Institute congratulates these Miller Fellows on their next endeavors:

Michael Abrams
Postdoc @ Harland Lab
Molecular and Cell Biology
UC Berkeley

Sam Hopkins
Simons Research Fellow, UC Berkeley (Fall 2021)
Starting January 2022: Assistant Professor
Department of Electrical Engineering and Computer Science
MIT

Ambika Kamath
Assistant Professor
Department of Ecology and Evolutionary Biology
University of Colorado Boulder

Nick Rodd
Staff Scientist
Department of Theoretical Physics
CERN

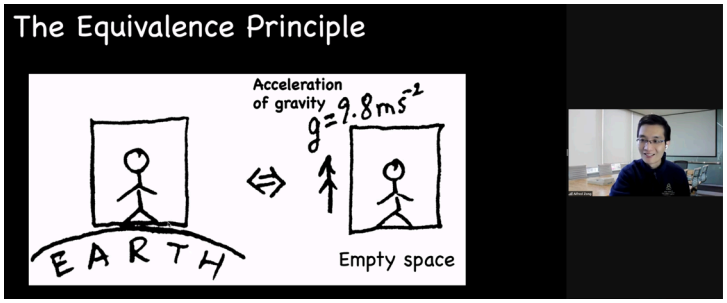


Yong Zheng
Assistant Professor
Department of Astronomy
Tsinghua University (Beijing)

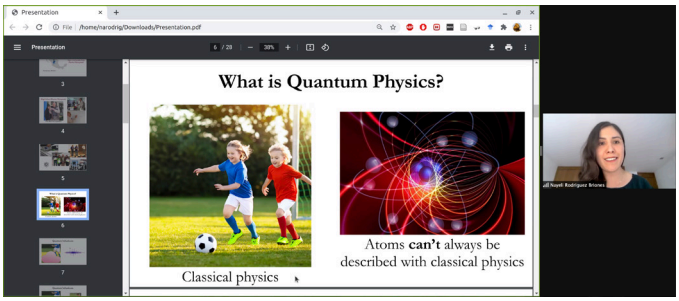
Miller Fellow Outreach

In the 2020-2021 year, several Fellows gave short presentations over Zoom to science students at El Cerrito High School with the goal of exposing students to career paths in science. Students in Environmental Science, Biology and Physics joined in. In each session, Fellows shared about their research and field, and answered questions from the students about the life of a researcher.

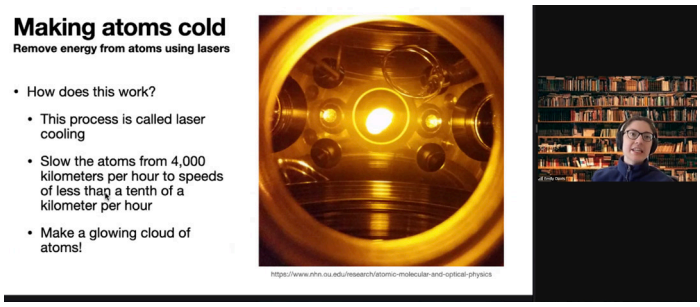
Big thanks to the organizers of this effort: Fellows Dan Ibarra, Yong Zheng, Nick Rodd and Gray Chadwick, staff member Vrinda Khanna, and El Cerrito High teachers Sam Nguyen and Elan Lavie; and a thanks to all the Fellows who participated in this program!



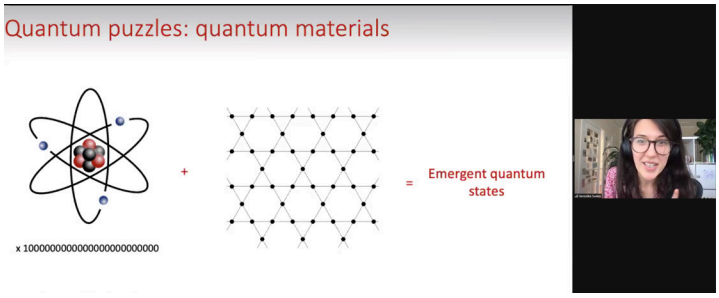
Alfred Zong, Miller Fellow 2020-2023, Chemistry



Nayeli Rodriguez Briones, Miller Fellow 2020-2023, Chemistry



Emily Davis, Miller Fellow 2020-2023, Physics



Veronika Sunko, Miller Fellow 2020-2023, Physics

Ekta Patel, Miller Fellow 2019-2022, Astronomy

Dan Ibarra, Miller Fellow 2019-2021, Earth and Planetary Science

University of California, Berkeley
468 Donner Lab
Berkeley, CA 94720-5190
miller.berkeley.edu

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miller_adm@berkeley.edu

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Thank you for your contributions!

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Mission Statement

The Miller Institute is *"dedicated to the encouragement of creative thought and the conduct of research and investigation in the field of pure science and investigation in the field of applied science in so far as such research and investigation are deemed by the Advisory Board to offer a promising approach to fundamental problems."*

For More Information:

+ Staff: Emily Birman, Donata Hubert, Hilary Jacobsen, Vrinda Khanna
+ millerinstitute@berkeley.edu | miller.berkeley.edu