Volume 42 Fall 2021

MURJ

Massachusetts Institute of Technology Undergraduate Research Journal

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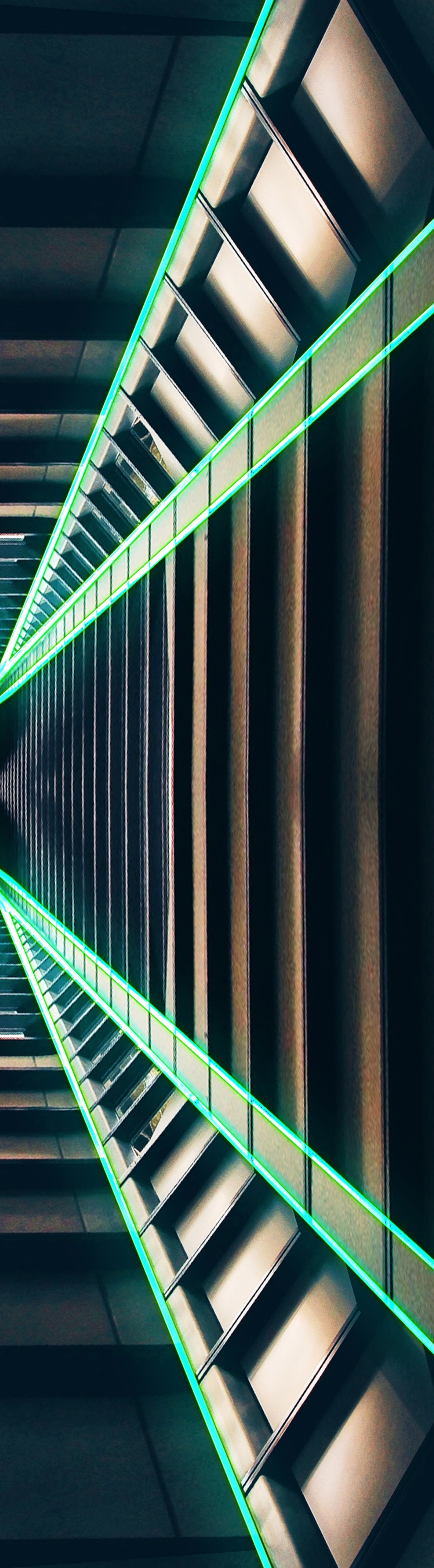
Community, Collaboration, Innovation

The Bayer Research and Innovation Center

Coming Soon to Kendall Square

*Science for a **better life***



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December 2021

Dear MIT Community,

As Fall 2021 comes to a close and IAP begins, we are delighted to present the 42nd issue of the MIT Undergraduate Research Journal. Throughout the past two years, we have taken part in countless experiences demonstrating the importance of community to science and of science to our communities. The MURJ team is proud and honored to continue in this spirit as we showcase the hard work, creativity, and innovation of our peers. This issue is published in honor of those who have sacrificed to protect their communities during this time. We are additionally grateful to the thousands of passionate and talented students across campus working to further knowledge in their fields, as well as the mentors that dedicate their time to training the next generation of researchers.

Enclosed you will find featured reporting on topics ranging from state-of-the-art quantum simulators, to AI-based heart failure therapy, to original commentary on the current state of life science research, to the study of ice fractures. Additionally highlighted are recent developments in MIT's outreach to high school students and the visions of Professor Gabriella Schlau-Cohen, who was recently recognized by the American Chemistry Society. Original student research published in this issue includes a biomimetic nanoplatform to aid the study of neurodegenerative diseases and a smart device and alternative compound to counter nicotine poisoning in real time.

As always, we acknowledge that the biannual publication of this journal is the product of hard work, collaboration, and commitment by MURJ staff members and often a product of years of

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hard work and investment by undergraduate researchers and their mentors. We would like to thank our editorial board and contributors for their time and hard work this semester and for persevering through the challenges of a largely remote school year. In addition, we would like to thank all the undergraduates who shared their research with us and the greater MIT community.

For previous issues of the MIT Undergraduate Research Journal, please visit our website at murj.mit.edu. If you are interested in contributing to future issues of the MIT Undergraduate Research Journal, we would be delighted to have you. Please contact murj-officers@mit.edu if you have any questions or comments.

Sincerely,

Gabrielle Kaili-May Liu
Editor-in-Chief

Massachusetts Institute of Technology

UNDERGRADUATE RESEARCH JOURNAL
Volume 42, Fall 2021

MURJ News

ARTIFICIAL INTELLIGENCE

Empallo: An AI Based MIT-spinoff to Watch

Innovators aim to create adapative heart failure therapy through artificial intelligence algorithms.

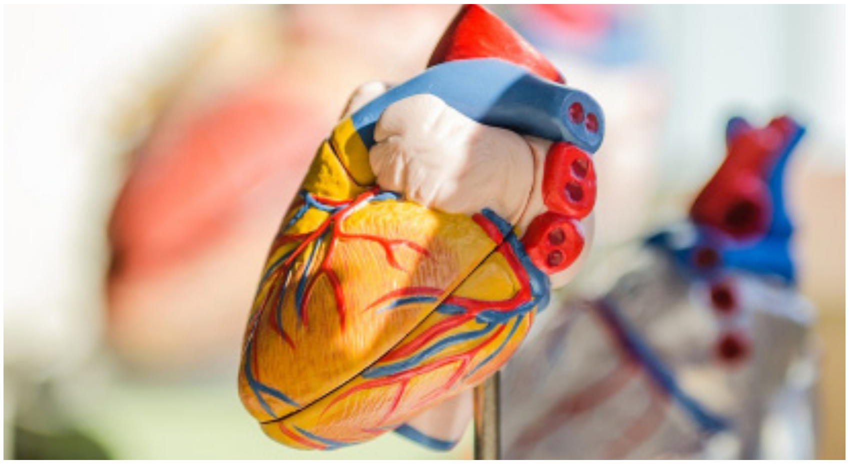
In September 2021, MIT's V Demo Day brought together budding university spun startups in culmination of the Martin Trust Center's delta V accelerator program. The teams showcased marketable innovations ranging from healthcare enrichment, to money transfer services, to social support platforms. Among the published list of 17 upcoming technological enterprises to watch is Empallo, a company started by Co-Founders Claire Beskin and Ray Liao. Beskin is currently an MBA candidate at MIT's Sloan School of Management who serves as Co-Managing Director of the university's $100K Entrepreneurship Competition, while Liao holds a PhD in Computer Science from MIT and works to develop machine learning methods and novel algorithms to apply to clinical problems. The company is additionally advised by Massachusetts General Hospital Cardiologist and EECS/Medical Engineering Sciences Professor at MIT, Dr. Collin Stultz, and has recently established partnerships with UCHealth, Mayo Clinic, and Beth Israel Deaconess Medical Center. But what does Empallo actually do?

"Half of all heart failure patients die within four years of diagnosis..." Liao contextualizes the complexity of long term heart failure treatment and remission in the United States during his delta V Demo Day talk. As he cites, 20% of heart failure patients are readmitted within a month of their discharge, and the US healthcare system spends $12 billion annually on heart failure hospitalization. Why is successful treatment of an increasingly prevalent disease (projected to increase by 46% by 2030!) so evasive?

"The fundamental challenge is the variability of this disease… When the patient is out of the hospital, the therapy has to be constantly adjusted for their dynamic and changing physiological state."

The issues, Liao explains, is that heart failure therapies are not customized and responsive to individual patient needs after their discharge from the hospital. As such, standardized at-home treatment plans fail to elicit long term remission across broad patient demographics. Empallo aims to enable the creation of adaptive therapy via artificial intelligence algorithms trained on electronic health records and other biometric data. The goal is for the algorithm to learn post-discharge disease patterns, to ultimately be able to "…predict clinical trajectories and recommend timely interventions." The algorithm can specifically be applied to guiding discharge readiness, medication planning, and home monitoring.

"The fundamental challenge is the variability of [heart failure] … the therapy has to be constantly adjusted."



With the expansion of digital record keeping in hospital systems, and growth projections for heart failure diagnoses, Empallo stands to make a lasting impact in the AI healthcare market. Liao and Beskin are currently working to market their service and establish new partnerships with integration health organizations and medical insurers. Learn more about Empallo at empallo.com

For a full list of "17 MIT startups to watch," check out: https://mitsloan.mit.edu/ideas-made-to-matter/17-mit-startups-to-watch.

— Prathysha Kothare

CHEMISTRY

The Award Winning Schlau-Cohen Chemistry Lab

Dr. Schlau-Cohen leads her team in cutting-edge biological and chemical research.

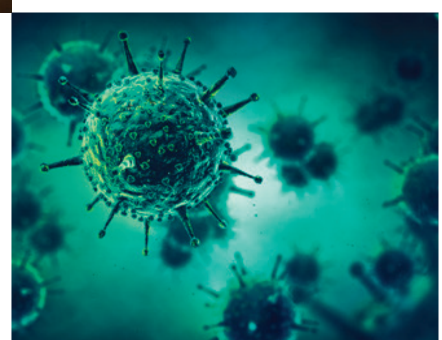
The American Chemistry Society annually recognizes the visionary and fundamental research of young individuals in North America through its Award in Pure Chemistry, and MIT's own Dr. Gabriela Schlau-Cohen has been named its 2022 recipient. With this recent distinction, Dr. Schlau-Cohen joins the ranks of brilliant researchers dating back 92 years to the award's inaugural winner and virtuoso of many trades, Linus Pauling. The prize is particularly dedicated to scientists with fewer than 10 years of experience since completion of their terminal degree, who have demonstrated "unusual merit" as well as "independence of thought and originality" in their chemical inquiries. So what exactly do Dr. Schlau-Cohen's seminal investigations concern? "… Lasers - Microscope - Proteins…" These lab website teasers are enough to elicit the curiosity of any scientific mind, and indeed the multidisciplinary research of Schlau-Cohen's team encompasses exciting applications across chemistry, optics, biology, and microscopy. She and her team of diverse graduate and post-doctoral students are particularly interested in applying the following methods, among others, to study biological light-harvesting and receptor protein systems, whose impacts range from improving solar energy technology to biomass production to medical therapeutics.

1) Ultrafast spectroscopy: Spectroscopy as a field concerns the characterization of spectra produced by matter or that which results from the interaction of matter with electromagnetic radiation. In this particular spectroscopic technique, an ultrashort pulse of light (with time durations on the order of 10^{-12} seconds) produces a broadband optical spectrum, and is used to study photo-induced events that operate on extremely short timescales. On a high level, these dynamics are captured by exciting medium with an ultrashort pulse, and thereafter probing it with a second light source to measure its absorption/emission profile over time. Several sub-methods exist within ultrafast spectroscopy, and Schlau-Cohen's lab has capitalized on these variations to describe energy flow, charge separation, and vibrational relaxation pathways that govern biological systems encompassing light harvest, chemical conversion, and membrane dynamics. Most recently, Schlau-Cohen's group developed a biohybrid photocatalyst to enhance the light harvesting capability and increase reactivity of photosynthetic systems under low energy irradiation! Read more about this work in their publication, "A biohybrid strategy for enabling photoredox catalysis with low-energy light."

2) Model membrane systems: Model membranes enable tractable investigations of specific properties and function of membrane components by isolating them in a physiologically representative yet simplified system. These membranes must be selectively engineered to express desired proteins, lipid composition, curvature, and stability. Nanodiscs are one such synthetic membrane system, and are composed of a phospholipid bilayer whose hydrophobic edges are screened by amphipathic proteins (i.e. membrane scaffolding proteins), peptides, or synthetic polymers. Nanodiscs offer high degrees of parametrization, ranging from lipid composition, disc diameter, surface area, disc stacking, etc. Schlau-Cohen's group employs these biological proxies to study membranous light-harvesting complexes and transmembrane receptors in vitro. The group simultaneously develops synthetic proteoliposomes with high membrane curvature and variable protein content to investigate higher order protein interactions. Just this year, the lab published findings that suggest the ability of membrane environments to tune the conformations and photophysics of light harvesting complex Photosystem II using fabricated nanodiscs and single molecule fluorescence characterization. Read more about the work, titled, "Membrane-dependent heterogeneity of LHCII characterized using single-molecule spectroscopy."

These projects exemplify but hardly do justice to the breadth, ingenuity, and ramifications of the Schlau-Cohen's lab research landscape. Since her appointment to MIT in 2015, Gabriella Schlau-Cohen has been bringing collaborative minds across STEM disciplines to branch into a vanguard of biological, energetic, and fundamental chemical inquiries. She will be presented the Award in Pure Chemistry at the ACS spring meeting in San Diego in March, 2022.

— Prathysha Kothare



MURJ Features

Arrange the Following Terms in Order of Importance:

Innovation, Funding, Applicability, Continuity

A brief commentary on the current state of affairs in the life science research ecosystem, narrated by its protagonists

By Arbri Kopliku

"And the most exciting part, even more than getting accepted to Nature Communications, is that it can get into clinical trials as early as next year," said Dr. Dan Goulet, postdoctoral research associate at the Koch Institute, during an informal interview this October. He was referring to his most recent co-authored paper on how IL-6 knockout mice exhibit a stronger immune response against acute lymphoblastic leukemia, and on how this finding can translate into curing human cancers.[1] As a curious but uninformed undergraduate I assumed that all great pieces of oncology research, much like this one, inherently contained a translational component that acted as the overarching motivation behind the project thesis in the first place. Seeing that my standards of evaluating research were slightly misled, Dr. Goulet went on to explain how the average shelf-life of research papers reaches almost a decade before they get dusted off and translated into the clinic. This sobering glimpse motivated me to better inform myself on the challenges that life science research at MIT faces on its path toward benefiting anyone besides the intellectual curiosity of the responsible scientist, and what determines its compatibility with the larger biomedical rebus of innovation. As I soon came to realize through my meetings with MIT professors and postdoctoral associates, it is all a matter of juggling time and attention between innovation in study approaches, procurement and retainment of funding, applicability of research outside the laboratory, and a guarantee that the project has a direction along which to keep growing.

My quest to better profile these components first led me to Dr. Bryan Bryson, Assistant Professor of Biological Engineering at MIT, whose lab studies everything there is to learn about tuberculosis pathogenesis and particularly engineering the host-pathogen interface as the infection is underway. His comprehensive answers very neatly fleshed out the research landscape that Dr. Goulet had sketched, despite studying as divergent ends of the human condition as offered by leukemia and tuberculosis. Funding is what allows ideas to turn into meaningful research, and according to Dr. Bryson it exerts undisputable influence on the paths chosen to address the more obscure parts of basic science. This unwelcome weight burdens the innovative approaches of the junior scientist much like it incentivizes the marginally incremental proposals of the senior one, thus propagating a complex interaction that reinforces itself upon ensuring the continuity of research work. While many Science, Technology and Society (STS) courses at MIT emphasize the deterministic role of innovation in motivating the natural course of research, funding turned out to be the most pragmatic lens through which to interpret Dr. Bryson's remarks, as well as to orient my following faculty interviews.

The biomedical research ecosystem conditions have to be exceptionally right for laboratory

1 https://www.nature.com/articles/s41467-021-26407-4

output to be taken up immediately by the field, said Associate Professor Michael Hemann of the Koch Institute, but there are lower-hanging fruits that scientists can aim at from the start of their experimental planning. Such is work in treatment protocols, where the individual drugs being studied have already been approved for safety and efficacy, as was the case with Dr. Goulet's group recommending the introduction of IL-6 antibody inhibitors earlier on in the ALL patients' drug regimens. Another potentially attractive field for fresh translatable research is that in diagnostics, and one in which Biological Engineering Professor Linda Griffith has extensive experience. She proudly summarized a good part of her research and advocacy career under the slogan "Endometriosis is not one disease," a strong argument in support of the importance that diagnostics holds in today's age of molecular characterization of disease. One of her many projects, a synthetic hydrogel, has seen an unprecedented spike in demand for use in human microenvironment modelling around the world, thus serving as a way of quantifying this gravitation towards diagnostics both in basic science and in engineering.

" Funding is what allows ideas to turn into meaningful research... it exerts undisputable influence on the paths chosen to address the more obscure parts of basic science."

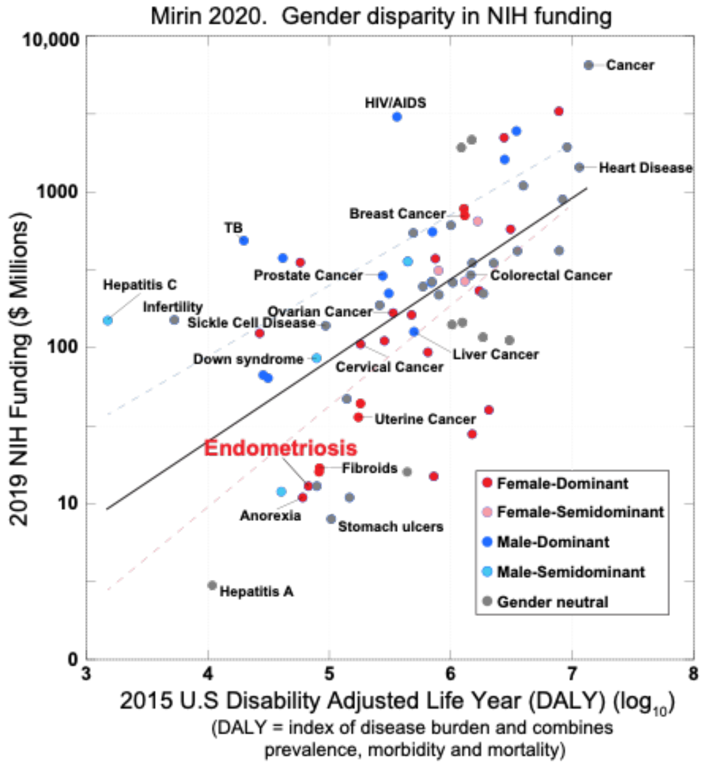
When it comes to funding, Professors Hemann and Griffith converged in their interpretations of where government funding for research currently goes: basic mechanisms are appreciated as the foundations holding the pyramid of progress in the field, but a hint towards future translatability is encouraged. One solution to this recurring obstacle, and one that rings closer to Dr. Bryson's own experience, involves coming up with research proposals that are daring enough to gain attention and consecutively funds even far from basic mechanism research. This risky approach has paid off in the past for Dr. Bryson, as his lab managed to pull money into tuberculosis work to develop the field's first CAR-T cells while competing with limelight oncology projects. The moonshot method is however quite unsustainable, as the gamble with such efforts by definition implies departing from the collective knowledge base and discontinuing that buildup of basic science expertise which could further delay applicable results in the statistically likely failure of the project. This is where the other biggest cash source in biomedical research comes in, the anonymous industry, which chases high risk – high reward opportunities to support undergoing projects from the successful proof of concept to the finish line, and that could sometimes get involved even earlier.

Professor Hemann's following dichotomy of industry funding aligned with the image that each interviewee portrayed when collaborations outside the academic research space were brought up. The first mode of industry involvement consists of grants for "generically funded science," which allow researchers to pursue their interests while helping the companies explore different aspects of cutting-edge science that could be of industrial interest in the near future. An example scenario is Prof. Griffith's group working on c-Jun kinase while closely affiliated to Merck KGaA in Germany, a prominent pharmaceutical actor. Despite the legroom that this pocket of cash provides for out-of-the-box research, its unsustainability arises from the misalignment of scientific curiosities between the lab and the funding company, often because of the difficulties in making a product out of a selection of papers. In this case, Merck soon gave up on their c-Jun kinase pipeline and licensed it out to a smaller company, which also failed to carry the project over the regulatory phases. The second mode of this academia-industry nexus involves companies hiring research laboratories to solve ultra-specific problems of the field, much like contract research organizations. This option of ambiguous intellectual appeal provides even less reliability for continued research, in the unlikely case that such a perfect motivational alignment

Picture 1: *We do not readily associate MIT life with science expertise, yet the iconic Great Dome is less than 1 mile away from Kendall Square, the figurative downtown to the biotechnology capital of the world. This close relationship makes the state of the complex biomedical research ecosystem an incredibly relevant aspect of the future of the MIT campus and its contributions to the field.*

is found. Academic labs in general, and more so at MIT, have a reputation for being pricey both in time and capital thanks to their publication-bound scientific rigor, which makes most of these contracts short-termed.

One could interpret the outline of this article so far as an argument against moonshots, and they would be right to some extent. The knowledge buildup principle to which I alluded while analyzing government funding assumes the validity of existing literature, but such assumptions on the other hand can interact unpredictably with the surrogate targets of young innovative scientists. In other words, our biotechnological era of single-cell RNA sequencing and flow cytometry underscores a responsibility coupled with sufficient power in individual researchers'



Graph 1.1: Courtesy of Professor Linda Griffith, taken from "Gender Disparity in the Funding of Diseases by the U.S. National Institutes of Health" by Author Mirin, Ph.D. (2020)

hands to re-evaluate the status quo of their respective fields, and this obligation extends beyond basic mechanistic principles. An interesting and rather complex example is that of combination therapies for blood tumors, such as acute lymphocytic leukemia (ALL): many of them were developed empirically from the observations of prominent physicians like Sydney Farber, the namesake of the Dana-Farber Cancer Institute, and have remained mostly intact to this very day. According to Professor Hemann, it is even more challenging to raise funds for the kinds of research projects needed to explore the mechanics behind such empirical treatment decisions, and that stems from the industrial disinterest in bedside deconstruction of the standard of care. Instead, most of the support goes for the homerun quest, for single drugs that will individually cure complex diseases, while we continue to serve chemotherapy patients cocktails including many drugs of different toxicities, just because trial-and-error concluded so half a century ago.

This discussion of the biomedical innovation ecosystem would be incomplete without mentioning how research work can indirectly shape the cross-sector interactions within the ecosystem and outwards to attain a self-promoting character. An illustration of this would be Professor Griffith's endometriosis work, and also the reason why a renowned authority in the scientific sphere flies across the country on a regular basis to advocate for broader attention towards "gendered" diseases. She says it is her duty to the field to use her credibility as Director of the MIT Center for Gynepathology Research, and not just her research output, to inspire other researchers to take on similar issues and counterbalance the inclination of larger players such as the NIH towards genomics and artificial intelligence, at a time when discoveries in diseases mostly affecting women could readily translate into the clinic. Professor Griffith referenced Graph 1.1[2] to outline the disparities of NIH funding with regards to gender and disease burden, but it also goes to demonstrate the variety of priorities given to biomedical research areas in general.

Overall, the relationships between innovation, funding, applicability and continuity of research invite deeper scrutiny to expose the complex life science research challenges faced on a daily basis that overarch the ecosystem as a whole. My discussions with MIT faculty and research staff touched upon different perspectives on the connections between these four broad terms, and how they ultimately affect lives outside of the lab. Very diverse issues were raised throughout the interviews, ranging from the inconvenience of clinical trials to workplace credibility, though most of them could be categorized into the four above-mentioned boxes and were shared in both basic science and engineering settings. This piece was meant to act as a peek into the immense food for thought within the biomedical research interface to better educate the scientists of the present and policymakers of the future, but it by no means does justice to the full picture. I want to thank all contributors for their time and insights which gave a unique flavor to each argument, while shaping my own understanding of the current biomedical research picture characterizations.

2 https://www.liebertpub.com/doi/10.1089/jwh.2020.8682

Quantum Simulators that Solve the World's Hardest Problems

By Ezra Yaador

In a research collaboration between scientists from the MIT-Harvard Center for Ultracold Atoms and other universities, a new programmable quantum simulator with a record-setting 256 qubit storage was constructed recently, in the latter part of 2020. This development makes a significant jump from what has previously been achievable in quantum devices of its kind by several times, marking a huge advancement for humanity in the race for quantum computing. For some perspective, before then, the largest functional quantum computers developed by tech giants IBM and Google, world leaders in quantum computing, were 53 and 54 qubits in size, respectively (5, 6).

"The hope is that there is something exponentially better or, at least, stronger than a classical computer."

For some background, qubits (quantum bits) are the classical computer bit ("0's" and "1's") analogs of quantum computers. However, instead of just taking on one "0" or "1" state at a time, qubits can be in a quantum mechanical superposition of those two states, or a "0" and "1" at the same time. A system of x qubits would yield 2^x complex coefficients or amplitudes, equivalent to quantum storage units. Therefore, while a system of 500 bits would yield 500 storage units, a system of 500 qubits would yield more storage than atoms in the universe (7). Because of the vastness of such quantum systems, quantum-based algorithms are suspected to be able to operate at speeds impossible for even the fastest supercomputers. Qubits are derived from various types of quantum particles and structures, such as trapped ions, photons, and optical lattices.

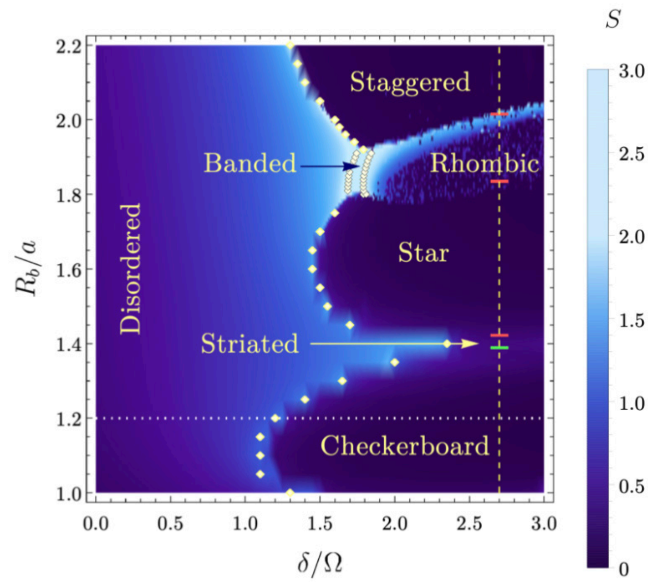
Quantum simulators are a special type of quantum computer that utilize, for example, laser-cooled neutral atoms (with superimposed atomic "spin up" and "spin down" states serving as the "0" and "1") to solve physics problems at the atomic scale. The applications of these simulators are more limited than universal quantum computers as computers are theoretically meant to do a variety of calculations, including those outside of physics. However, quantum simulators can prove to be superior as they can solve many major scientific problems that quantum computers, due to their lack of well-controlled, error-corrected qubits of sufficient quantum volume, are decades away from solving (2). Therefore, quantum simulators, rather than all-purpose quantum computers, may serve to provide the "quantum killer app" that many have been seeking to facilitate humanity's advancement into a world of quantum technology. As a result, QuEra, a quantum computing startup founded by the researchers that is launching accessible versions of their simulator by 2021, has already raised $17 million from investors, including Tokyo-based e-commerce company Rakuten, and generated $11 million in revenue (4).

In an earlier collaboration in 2017 that included Professor Vladan Vuletić, a co-developer of the new simulator and co-founder of QuEra, the team constructed their original version of the device with a storage exceeding that typically produced at the time: 51 qubits. They utilized ideas known at the time but believed not to work very well, but according to Professor Vuletić, the entire process worked magically well.

"So before, people could already trap individual atoms into individual traps, but only with about 50% probability. That made it so that if you have a large system of 10 or 20 or 50 traps, you would hardly ever exponentially fuel instances where you trap all of the atoms." However, Vuletić and his team discovered that, after randomly loading atoms into the array, one can look at which array positions on the 2D quantum simulator are filled with multiple atoms and, from that, redistribute those atoms to quasi-deterministically load one atom per trap. "It's really this trick at the moment that works rather well."

However, in this latest discovery, the scientists utilized a more efficient protocol which enabled them to move entire rows of atoms in parallel with two sets of movable optical tweezers, or lasers. Multiple moving traps aligned in parallel enabled multiple atoms to be moved up their respective columns at once, creating the much larger 2D arrangement of atoms. As stated in their paper, the entire process only takes 50-100 milliseconds with more than 99% of the array filled.

In their paper, the researchers used the device to study quantum phases of matter: a star phase, a striated phase, and a checkerboard phase. These phases arise from the atoms adopting lowest energy conformations in the array when their interactions are increased to certain strengths, analogous to, for example, liquids conforming to solid crystals at certain temperatures and



Quantum phase diagram with phases studied by the simulator from a previous paper. The axes represent parameters for the atoms' interaction strengths. At certain interaction strengths, the atoms transition from disorder to the various phases. Used with permission from (7).

pressures. However, the atoms' behavior in some phases, such as the striated phase, cannot be explained by just classical particle, or crystal, dense-packing; their 2D alignment arises, in part, from quantum fluctuations. In between the phases, the scientists were able to observe quantum phase transitions for the first time ever, specifically in the Ising (2+1) dimension (2D plus time dimension) universality class. The Ising Model serves as the benchmark model system for studying phase transitions in both classical and quantum matter; it's essentially the Drosophila fruit fly of physicists (3). Therefore, with their discoveries, the researchers made significant contributions to studies of quantum many-body

"Already, the simulator has allowed researchers to observe several exotic quantum states of matter that had never before been realized experimentally, and to perform a quantum phase transition study so precise that it serves as the textbook example of how magnetism works at the quantum level." -The Harvard Gazette

behavior that have implications for quantum material and device optimization.

A significant feature of the simulator is that it can be used to conduct fundamental research and directly study quantum phenomena in all types of processes. For example, in chemistry, the device can directly emulate molecules and chemical reactions, and it can even determine whether the products of a reaction can be modified just by manipulating the wave functions (particle-wave duality) of the same starting materials. In biology, the simulator will be able to reveal the role of quantum effects in photosynthesis. In general relativity and cosmology, the simulator can be used to study various theoretical phenomena, such as quantum effects in curved spacetime, by simulating them, and when combined with high-precision measurements, it can even be used to detect and study gravitational effects. In quantum transport, it can create and simulate quantum complex networks, including models of a future quantum internet.

According to Professor Vuletić, elucidating the scaling behavior of certain quantum studies and computations were one of the main motivations for the quantum simulator expansion.

"Quantum computers, as they work right now, won't be better than classical computers, but we're interested right now in how they scale," he says. Studying scaling behavior would shed new light on how fast quantum computers can do certain calculations, and it would show how much advantage qubits have over classical bits as a computation becomes very large.

"The hope is that there is something exponentially better or, at least, stronger than a classical computer."

One of the biggest challenges moving forward in designing quantum computers, he says, is in their storage encoding.

"In a classical computer, we encode bits redundantly, meaning we make several copies of the same memory bit, and if one of them gets lost because, you know, a high energy particle flies through your computer, you still have the other copies and can correct any errors that happen."

However, in quantum computers, this is much harder to do. Merely looking at the state of a quantum bit, for example, would actually destroy a part of it (due to quantum decoherence); instead, one would have to compare pairs of qubits and, from that, derive their states. The analogous method of error correction in quantum computers, termed Quantum Error Correction, has been theoretically proven to work, but no one has fully demonstrated it in a quantum computer yet.

"With the current schemes, we would need many, many quantum bits to encode just one logical, protected quantum error code."

With a developed protocol for quantum error correction, the researchers, along with others, will eventually be able to develop universal quantum computers of larger scale that can solve the world's outstanding scientific problems. However, quantum simulators are taking on that role right now, and they, actually, may be the quantum devices that facilitate humanity's advancement into a world of quantum supremacy.

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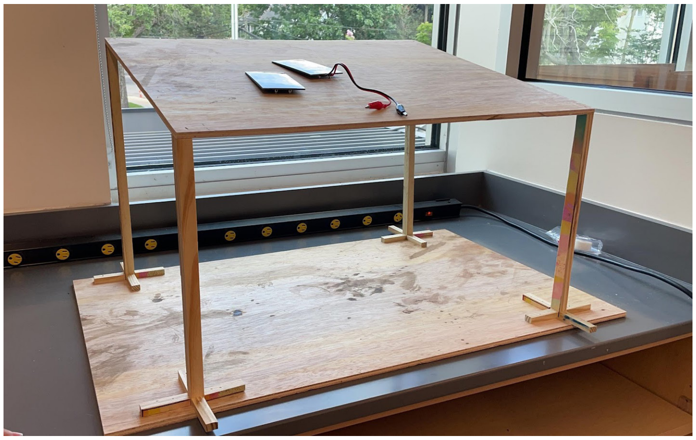
(11) Interview with Professor Vuletić

An Exciting Outreach Opportunity: Expanding MIT's Connectiveness with High Schools

This issue's spotlight features Ed Moriarty and Chris Mayer

By Lia Bu

Before Mr. Ed Moriarty, an instructor at MIT's Edgerton Center, concluded his mini building workshop offered to accepted students during the CP* week, he offered an interesting opportunity to those in the Zoom call. To those interested, he and Mr. Chris Mayer, the clubs and teams liaison, proposed an idea that revitalized and expanded the impact Global Teaching Labs (GTL) have on their students. Due to COVID-19, the limited travel impacted this program. Therefore, Mr. Ed Moriarty's alternative solution included accepted students to MIT (and therefore incoming first years) could develop and run an engineering design workshop (EDW) program that allowed the first-year's high schools and the Edgerton Center to connect and explore teamwork and design projects. Out of the 20 or so in the first Zoom call, the collaboration solidified to include Victoria Velazquez, Grace Jau, Catherine Tang, Abitha Vegi, Yitian Zhu, Sarah Lu, and myself (Lia Bu). Out of 6 people, there were four high schools that participated in this program: Seven Lakes High School (Katy TX); Mission San Jose High School (Fremont, CA); Hialeah Gardens High School (Hialeah Gardens, FL), Woodside High School (Woodside, CA), and Isidore Newman School (New Orleans, LA). Each of the four teams developed a team or teams of students that led projects ranging from 3-4 weeks of the program. To encourage collaboration, all the schools began with a fun activity: launching water rockets! This activity encouraged a team-working dynamic that served well when the main projects ideation



The Initial Stand

process rolled around in the second week of the program. Each team additionally had sophomore mentors in addition to the rising first years connecting back to the Edgerton Center and MIT's resources.

Developing this project at my high school (Isidore Newman) included many different moving parts. In April and May, I attended weekly meetings that allowed first-year students and me (named FRED) to develop this program, and to build leadership skills. Within my school, I worked with Mr. Matthew Jones, the head of the science department, and Dr. Andrew Hermann, the chemistry teacher. We all were very excited to see how the program would turn out, and began the program around a week early to meet with the team and begin to generate ideas for potential projects.

In our first meeting (after the team-building rockets), both Mr. Moriarty and Mr. Mayer wanted to encourage crazy team building ideas, even if they weren't feasible. The four students participating in the program scampered around the room, writing down random ideas on sticky notes and organizing them on the white board. My personal favorites included a painting soundscape, which could transform images into sounds, a solar-powered car and stove, a Stirling engine generator, a smart bike stand, and an interactive game. These ideas were taken apart, smushed together, and completely transformed in a way I didn't think was possible. Watching the team interact in generating these ideas using their imaginations and creativity was amazing and demonstrated that teamwork is crucial in any design process, as the best ideas from my team came from throwing around random concepts.

As a result of this two-day ideation process resulted in two main projects that were pursued, along with individual work. The side project that two out of the four team members pursued included building a 3-D game of clue. Building upon an original CLUE Board, they envisioned building a house on top of the foldout and making it so that the piece travelled in a three-dimensional space, adding to the complexity of the game. Using both CAD modeling and hand-drawn plans, they truly improved on the game, even by changing some of the rules to make it fairer. Unfortunately, the laser cutter was unable to be used until the beginning of the school year, but the foundation of the project was completed successfully.

The big project that all four team members pursued came from a mash-up of the "smart bike stand" and the "solar-powered car." The team thought, "why not put them together?" Therefore, the team quickly began to pursue a solar-powered charging station for e-bikes, that would sit on Isidore Newman grounds able to be used by any member of the community that commuted with e-bikes to school.

Since this was such an expansive project (as we were building it from the ground up, no pun intended), there were initial doubts on its feasibility. However, I believe that my team was particularly suited to this project. Each of the four members was knowledgeable of a certain part of the project. For example, one handled electronics, as he was very invested in batteries, currents, and wiring. Another handled the design and the modeling of the structure, as he was experienced in CAD modeling and design. The other two members wanted to learn more about woodworking and the construction of the project, and so they contributed significantly, along with the others, to making the physical prototype and the building of the physical structure. All three different fields played off of each other very well, creating this hub of designing, pushing ideas, and innovative solutions to problems that we ran along into the way.

During the beginning of the thinking of this project, the team did research, calculations, and compilation of the materials that might be necessary. We first began with a prototype of the stand. The prototype initially consisted of a

The Building of the Structure

rectangle platform laying on 4 legs (like a table) but was slanted around 15 degrees (so that one pair of legs was lower than the other). On this slant, the solar panels would lay to catch the solar rays. We had not thought of where the box holding the necessary electronics would go, and we did indeed run into this situation later in the main building process. To support the legs, there was cross bracing on the bottom, acting as feet.

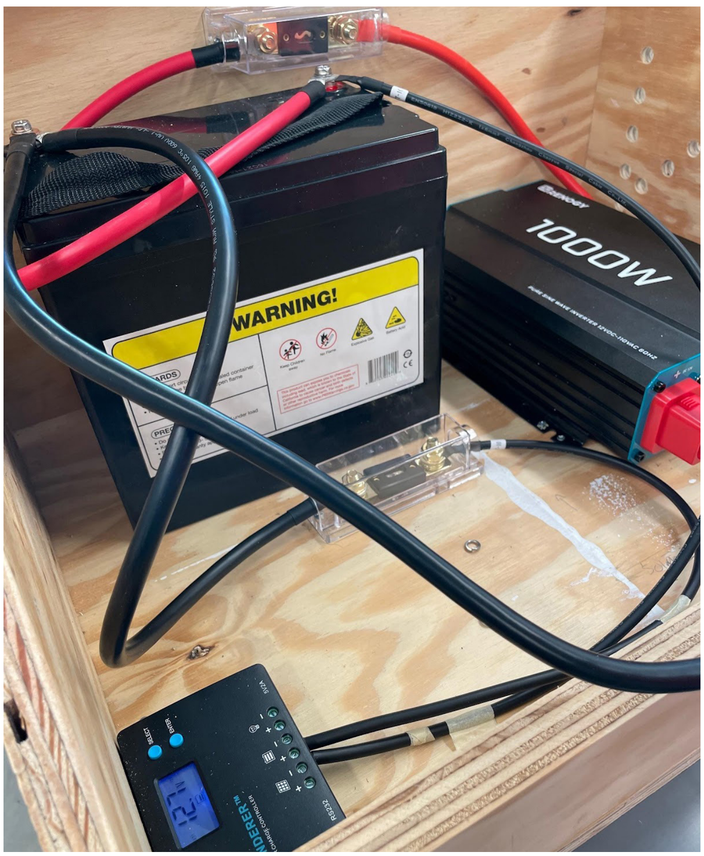
"The big project that all four team members pursued came from a mash-up of the 'smart bike stand' and the 'solar-powered car.'"

When the team proposed the idea to Mr. Moriarty and Mr. Mayer, it was clear that there were critical design challenges in the proposed build. Firstly, the 15 degrees were not sufficient to catch all of the rays possible, missing out on the maximization of the solar charge. Based off the latitude of New Orleans, the roof of the panels needed be 30 degrees slanted. Secondly, to make this a sound structure, the design needed cross bracing not on the feet of the structure, but on the legs (making an X across the smaller and longer legs). We additionally would need extra 2 by 4's to stabilize the roof, so that it could hold up the solar panels. The team designed this structure in mind to withstand very strong winds New Orleans, and so the design needed to be completely stable. Our sophomore mentor, Charles Bales, is an architecture major, and so he made very insightful comments to improve the build.

A critical member of this team not originally part of the project was the school's Technical Theater Director, Mr. Philip Cramer. Without his knowledge and guidance of construction, the project would not have been possible. He additionally provided comments that were additionally helpful, as he was there in person watching the construction and providing real-time feedback.

The team went back to the drawing board, but additionally, during this time, the electronics required also began to be drafted. Because I was

purchasing the necessary materials, I worked closely with Mr. Jones and the team member focusing on electronics. We eventually settled on a system that greatly eased any unnecessary work required on the circuitry and made it safe: we purchased mostly Renogy products. This eased the circuitry, as we did not have to spend time figuring out if different devices from different companies were compatible with each other. However, we did have to buy the wires separately due to shipping delays. We did unfortunately run into the zone of waiting for materials, but this was remedied by watching science videos and pursuing quick projects, such as the construction of a model airplane and expanding on the 3D-clue project.



The wiring of the electronics box

However, once the supplies all arrived, it was crunch time! The team originally met for four hours each day during the weekday, but this sometimes stretch to five hours as there was a lot to accomplish. The team started by constructing the main frame of the build. Cutting around seven and nine feet of 2 by 4's was challenging, but with Mr. Cramer's and Dr. Hermann's directive, the team accomplished the main frame in around 3 days. This included using carriage bolts for the frame, which theoretically would allow for quick dismantling of the structure in case there was a hurricane about to land. This wasn't the case, however, and the structure was so large and heavy that it was very hard to put up and take down and put up again. Therefore, we no longer worried about truly taking it apart after it was built for the last time. All four contributed to painting the primer on the wood and letting it dry. Around this time, we ran into the technical challenge of storing the electronics safely.

The biggest concern about the electronics (which included a solar charge controller, a battery, and an inverter) was storing it safely. Outside, the electronics would be subject to the elements and any critters it might encounter. While our first idea was to place a weatherproof box in the corner, the team quickly realized that the electronics were quick to get hot, and that they ran a chance of overheating in a closed box. However, placing mesh on the box was extremely difficult, as the box was designed to hold only the electronics, minimizing as much space as possible. As a result, the team bolted it to the underside of the roof. This was extremely successful (although difficult, as the box weighed around 40 pounds)! For the circulation of air, we drilled holes in shape of an N for Newman and painted in green, so that it was visible to those that used the bike station or passed by it.

When we were finally ready to build it outside (as it was so large it couldn't fit through the doors or on the truck) the team enlisted the help of their parents. Their parents dropped by at one time or another, one of them bringing supplies for the project with her. Another helped us lift the massive 2 by 4's and the ten feet by four feet roof onto the platforms. At times, it was excruciating to work in the 95-degree heat, with the sun barreling down as we worked in the afternoon (we had to then move it to earlier in the day to finish the project). I could feel the camaraderie in the air as we worked to finish the project with both the team members and their families.

We spent the next few days painting it, hooking up the solar panels, and wiring the circuitry together. A team member additionally added further artistic details to the frame. He painted green stripes down the cross-bracing, adding a nice pop of color to the frame. (The green and white refer to Isidore Newman's school colors). As a result, it fit in perfectly with the theme of the school and its location next to the football field. An added benefit of the project the team thought of included its use when not as a bike stand. During games, it could serve as cover for the ticket stands and would allow people to charge their phones or other devices off the solar power.

With the succession of the project, the last final push for the team was to compile all their work for the month and create a presentation. During this time, we were able to hear about the projects from the other schools as well. For example, from California, my team heard about how it was like to design unique games, and their experiences with the bottle rockets. When it came time for Newman to present, my team did it smoothly. Detailing both their challenges and success that led to the completion of the project, some of the biggest takeaways for the team members included exploring working on a team well with a big project, learning about different types of engineering, and being exposed to the building and woodworking process. Both Mr. Moriarty and Mr. Mayer were proud of the work, as was I, for the work and learning the Newman team did throughout the summer. The team was able to break down an idea that seemed overwhelming into an extremely successful project that charged a computer, a power tool, and is currently used by the faculty at Newman who utilize e-bikes.

As for myself, I learned during the summer how to lead a team of different personalities, interests, and experiences towards a common goal. Interacting on problems has helped me transition to MIT, and the collaboration I did with my fellow classmates and the Edgerton Center gave me a change to adjust quickly to my first year at MIT. Regarding my team, I offered advice when I could, compiled information, and proposed solutions. However, this project was truly team-drive by the high schoolers, and it was phenomenal to see not only the project's growth, but their growth as well in learning how to think, problem solve, and use their imaginations. Reflecting on the program, starting from a CAD design model to an actual structure that currently stands tall at Isidore Newman School seems mind-boggling. However, with the help of Dr. Hermann, Mr. Cramer, Mr. Jones, Mr. Moriarty, and Mr. Mayer, and Charles, my team worked very effectively for four weeks and were able to produce a project and a program they and Newman can be very proud of. I cannot wait to hear about what they do in the future as they continue to grow and use the skills learned in the program.

Cracking a Path Forward: Ice in the World of Fracture Simulation

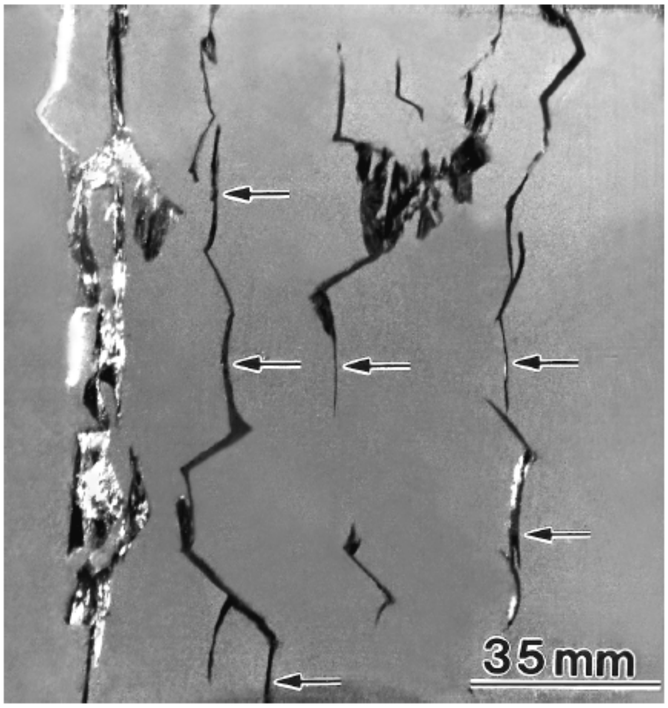
By Hillel Dei

“We cannot ignore the vital role of ice in the ecological system, in the polar caps, and in moderating the global climate”

Ice. You know what it is. I know what it is. You’ve played with it, used it to freshen up your beverages, used it to soothe injuries, and may even now be doing something with it as you read this article. You might even be listening to, “Ice, Ice, Baby.” Then, we cannot ignore its vital role in the ecological system, in the polar caps, moderating the global climate. But here’s one thing I bet you’d never have considered. Have you ever looked at ice and thought: Hey, let’s use this as the basis of a new modelling system? Have you ever watched your ice fracture, and then imagined setting up a series of experiments in collaboration with the United States Government to try to anticipate how cracks propagate within ice, and use this as a building block to anticipate how cracks behave in general? I’m guessing you, oh reader mine, did not yet imagine having done that. Allow me, to introduce to you, the wonderful world of fracture simulation.

Let’s begin by turning back the clock to provide some historical context. From 1944 to 1961, the research agencies known as the Frost Effects Laboratory, SIPRE (Snow, Ice and Permafrost Research Establishment), Arctic Construction and Frost Effects Laboratory (ACFEL) were established. This subdivision of the U.S. Army Corps of Engineers conducted research, as I am sure you can imagine, around ice and frost: from means of construction in cold regions to how best to transmit signals in this extreme terrain. From the chemistry within soil in extreme terrain to tracking water bodies. Anything ice-related was done by these groups, which has evolved over the years into the organization currently known as CRREL (Cold Regions Research and Engineering Laboratory) and still a close affiliate of the US Army. With this historical context in mind, we may appreciate how a collaboration was struck between the fine engineers of MIT and the snowmen of CRREL, with both being highly research-intensive organizations and CRREL’s projects easily aligning with MIT's mission toward the betterment of mankind.

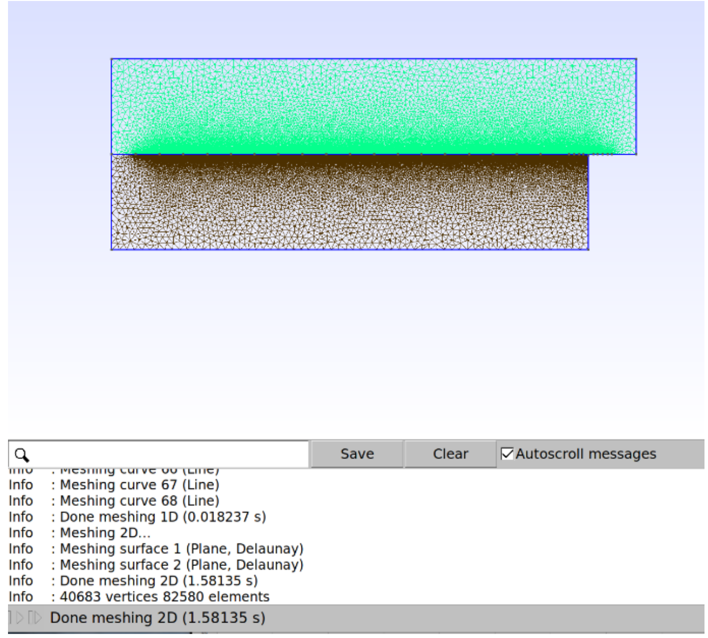
The phenomenon of ice cracking had long been a well known one. I mean gosh, just chew on ice picks and you’d easily observe it. It was also understood that the unique nature of ice—which permits easy identification of cracks, simple control of experimental errors through increased trials, elastic behavior that obeys Hooke’s law over a reasonably large area (meaning plots of its load-displacement curve would be reasonably consistent), and remarkable cohesion while cracking—makes it the ideal candidate. In this context, an experimental plan was put forth, and MIT’s partners at CRREL decided to conduct the following experiment: a sheet of ice, bound to a thin slab of aluminum as illustrated below, would have some force applied to it. This would induce a shearing effect and a plottable load displacement graph that could easily adopted for modeling. In other words, this would give us a reasonable goal and a specific target to work toward: an experimental value to chase, if you will.



Source: E.M. Schulson; *The fracture of water ice: A short review*

Now comes the fun. With the experimental results in hand, we were tasked with creating a simulation of the ice fracture. Allow me to put this in context. MIT, or more specifically the Radovitzky Research Group, was tasked with creating a software simulation of the ice fracturing experiment that reproduced, or came reasonably close to reproducing, the physical cracks induced.

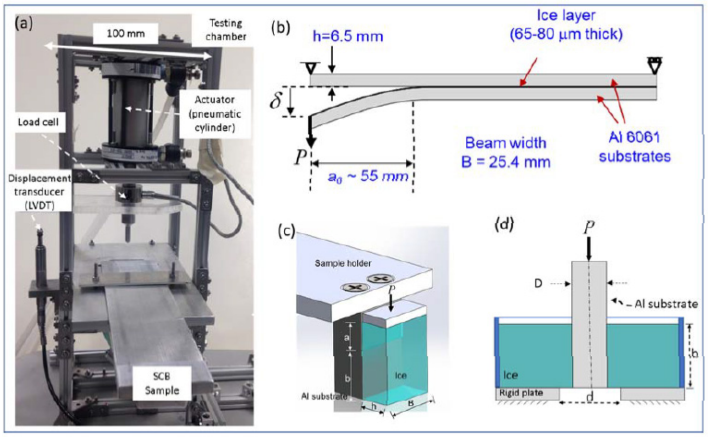
To provide a massively oversimplified explanation of the tools used in simulation: MIT researchers constructed a software package in which a facsimile of the structure of ice was constructed using a triangular mesh (an example of the generation process is given in the image to the right above). The size of this mesh could be altered to increase or decrease the number of triangles within it. The program functioned by performing calculations at each time-step, such that the parameters used in calculation could be modified. Thus, other possible alterations included changes to typical material properties like Griffith Energy, elastic modulus, and Young's Modulus, among others. This variety allowed for significant versatility in simulating the behavior of ice: simulations could be run repeatedly with alterations to the mesh and material properties, in order to achieve a closer match with the



Example of the mesh generation process

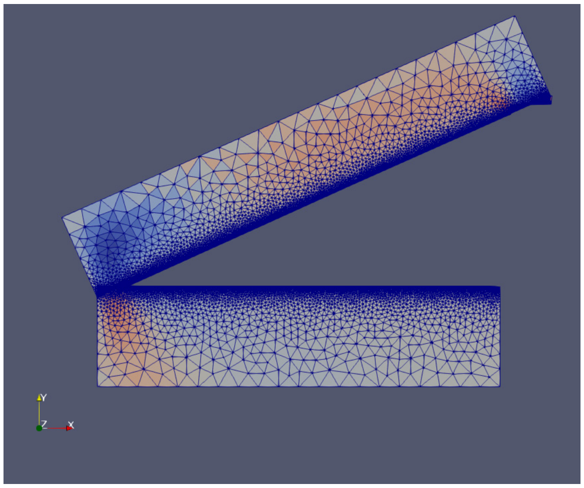
experimental properties observed.

Given this setup, the software could permit a crack to propagate: the load and energy travelled along the ice-aluminum boundary with the result of each successive stage based on the outcome of the previous time step until the energy had been sufficiently dissipated, or until the crack had fully propagated and the two materials were separated. For confidentiality, I cannot divulge the actual models used. However, the publicly available experimental results shown below will serve just as well to help us visualize the experiment performed, and the results we sought to approximate:



Source: Dawood; Characterization of Ice Adhesion: Approaches and Modes of Loading

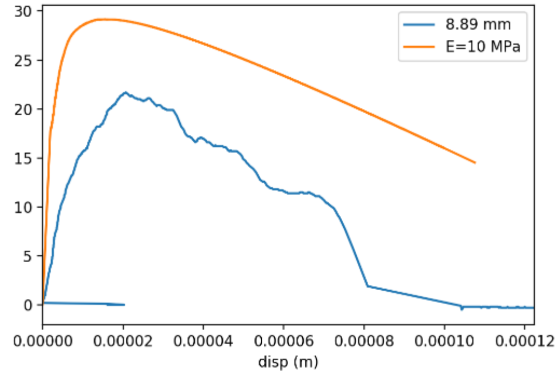
Depicted below is an example simulation of the ice fracture experiment. To learn more about the specifics of the math involved, and how the simulation kit was created, please refer to the following paper by Professor Raul Radovitzky: “A scalable 3D fracture and fragmentation algorithm based on a hybrid, discontinuous, Galerkin, cohesive element method.”



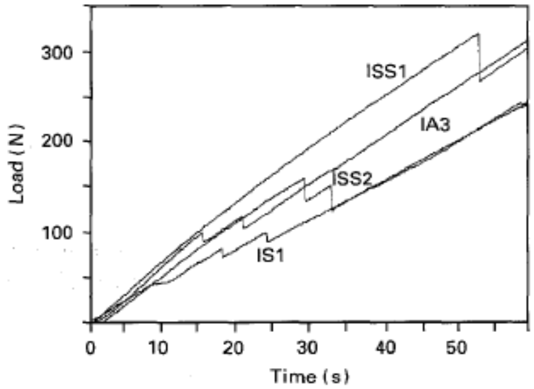
With the aforementioned goal in mind, let us now proceed to examine the extraordinary progress made in this research; this is easiest done by comparing the simulated load-displacement curves with the experimental results obtained. After months of improvement, our results came extremely close to the experimental observations, and this was no easy task.

In addition to the following graphs, the first image on the subsequent page effectively summarizes the essence of this project: at each time-step, based on the methodologies used by Radovitzky et al., calculations were iteratively performed to determine from the results of previous time-steps the load and then the displacement. This permitted creation of a model of how the crack propagates. Parameters were pulled from a material data file for simulations.

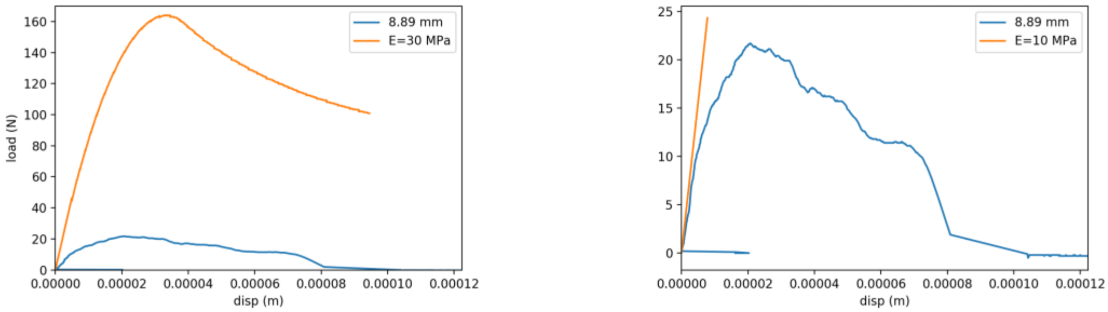
In my experience, the single greatest problem we faced, and one of the earliest problems, in fact, was the violation of the constitutiveness



Depiction of one of the more recent load-displacement curves, with the blue line representing the experimentally derived trajectory and the orange line representing the theoretical trajectory.

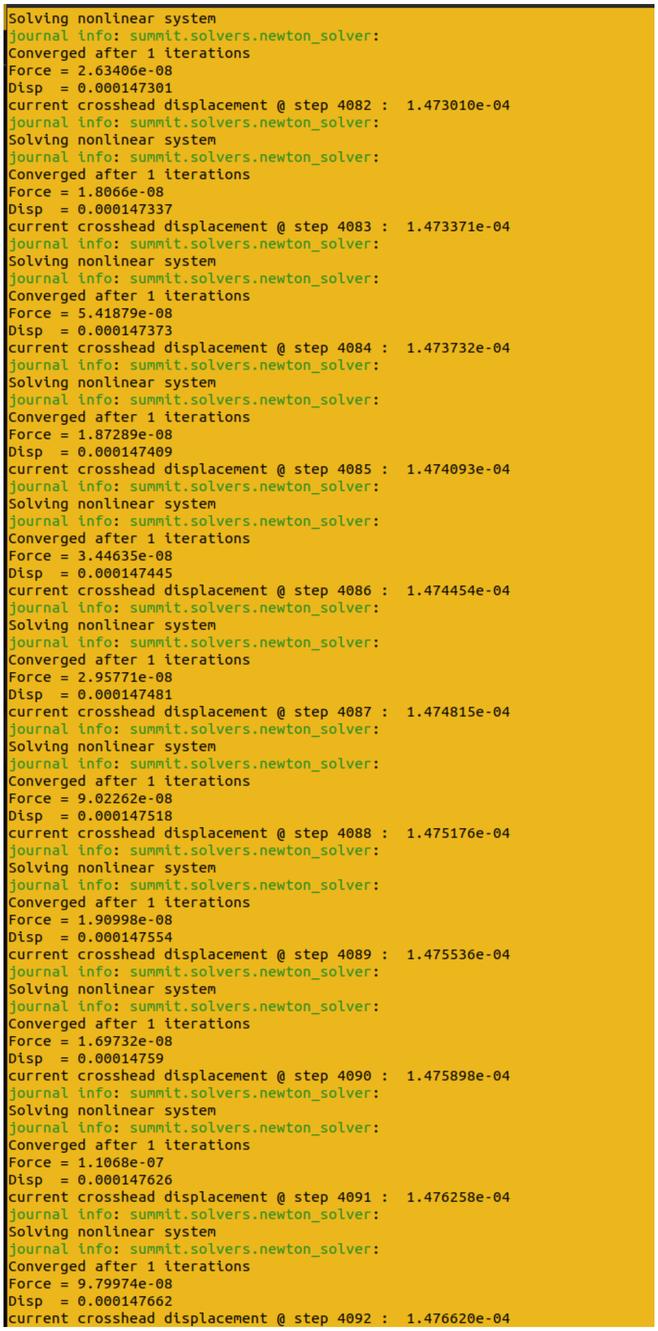


Example of a typical load-time curve as opposed to load displacement, again used in lieu of confidential results. Source: Y. Wei; Ice/metal interfaces: fracture energy and fractography



E=30 MPa E=10 MPa

Depiction of the extent to which varying the material parameters can affect the results yielded by the simulation kit



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Converged after 1 iterations
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Disp  = 0.000147301
current crosshead displacement @ step 4082 :  1.473010e-04
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Solving nonlinear system
journal info: summit.solvers.newton_solver:
Converged after 1 iterations
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Disp  = 0.000147337
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Converged after 1 iterations
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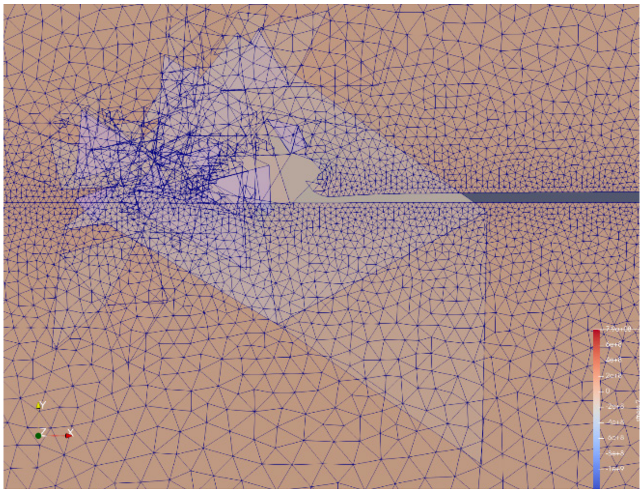
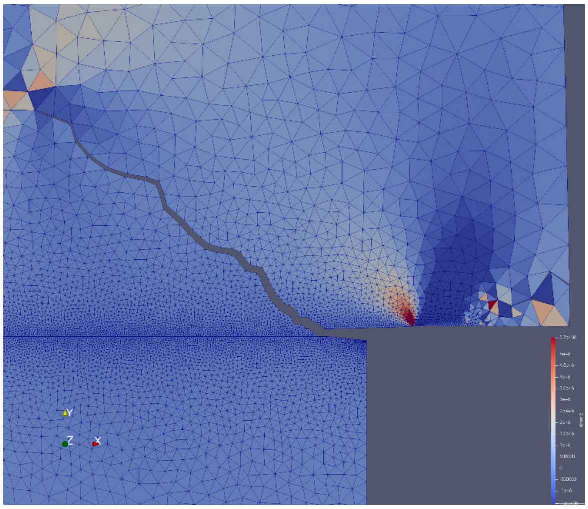
property. In simple terms, this property means we cannot have two entities existing in the same spot at once. We unfortunately ended up with this exact problem, indicating that our results needed fixing. The image to the right above depicts a sample mesh output by our simulation kit for which the constitutiveness principle is clearly violated. To address this problem, we utilized a redesigned mesh in which the triangle looping path was altered and a three-layer mesh was created. As there would be an extremely thin layer of aluminum oxide between the ice and aluminum, this intermediate layer could act as a buffer against more extreme conditions.



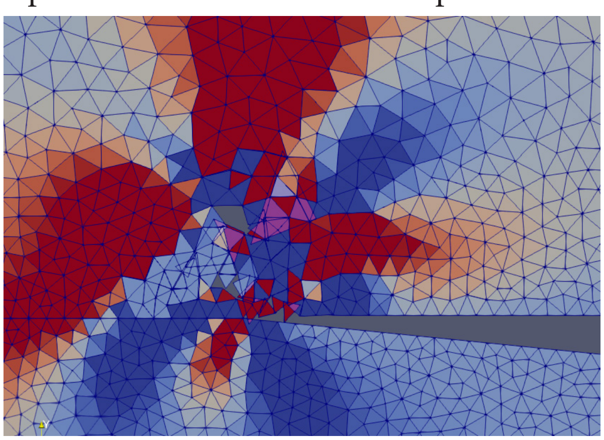
The next failure case encountered was mesh disintegration. To provide an illustration of this: please consider the difference between ice and snow. If you were to take a blade and cut through ice quickly, it would split into 2 pieces while still retaining its shape. Contrast this with snow, for which the same procedure would cause an almost explosive effect in which the snow falls apart. Intuition predicts that ice would not behave in this manner. Yet according to the results of our mesh, this was indeed the case. To resolve this issue, careful adjustment of the aforementioned material parameters was required.

Following this challenge was a case of inconsistent elastic behavior. To provide a bit of intuition from the real world, allow let me ask a simple question. Have you ever seen ice bend? No? Me neither. The results of our simulation seemed to differ, and resolution of this error required research into acceptable material parameters which we could justifiably claim to use in our simulation, along with a reworking of the mesh loop, which eventually was, too, resolved.

To explain the third challenge encountered, it is easiest to explain the solution first. Increasing the interface energy made it more difficult for the crack to propagate into the ice itself and not along the boundary. In other words, the crack was expected to move along the interface between the ice and aluminum, but curiously it propagated into the ice, as shown below. To solve this, we increased the interface energy until there was no way a crack induced by force of that order could penetrate into the ice, and when the latter issue resurfaced at a subsequent time, it was easily addressed by the three-layer mesh, since the aluminum oxide layer between the ice and aluminum was uniquely set up to prevent the crack from breaking into the ice.



The final challenge encountered was the curious case of chipping, depicted below. Effectively, holes were being created within the mesh as the crack propagated, and this was more of an amalgamation of prior problems: the crack's propagation into the mesh and the mesh's own failure to remain intact. As such, the solution to this problem was the sum of all prior solutions,

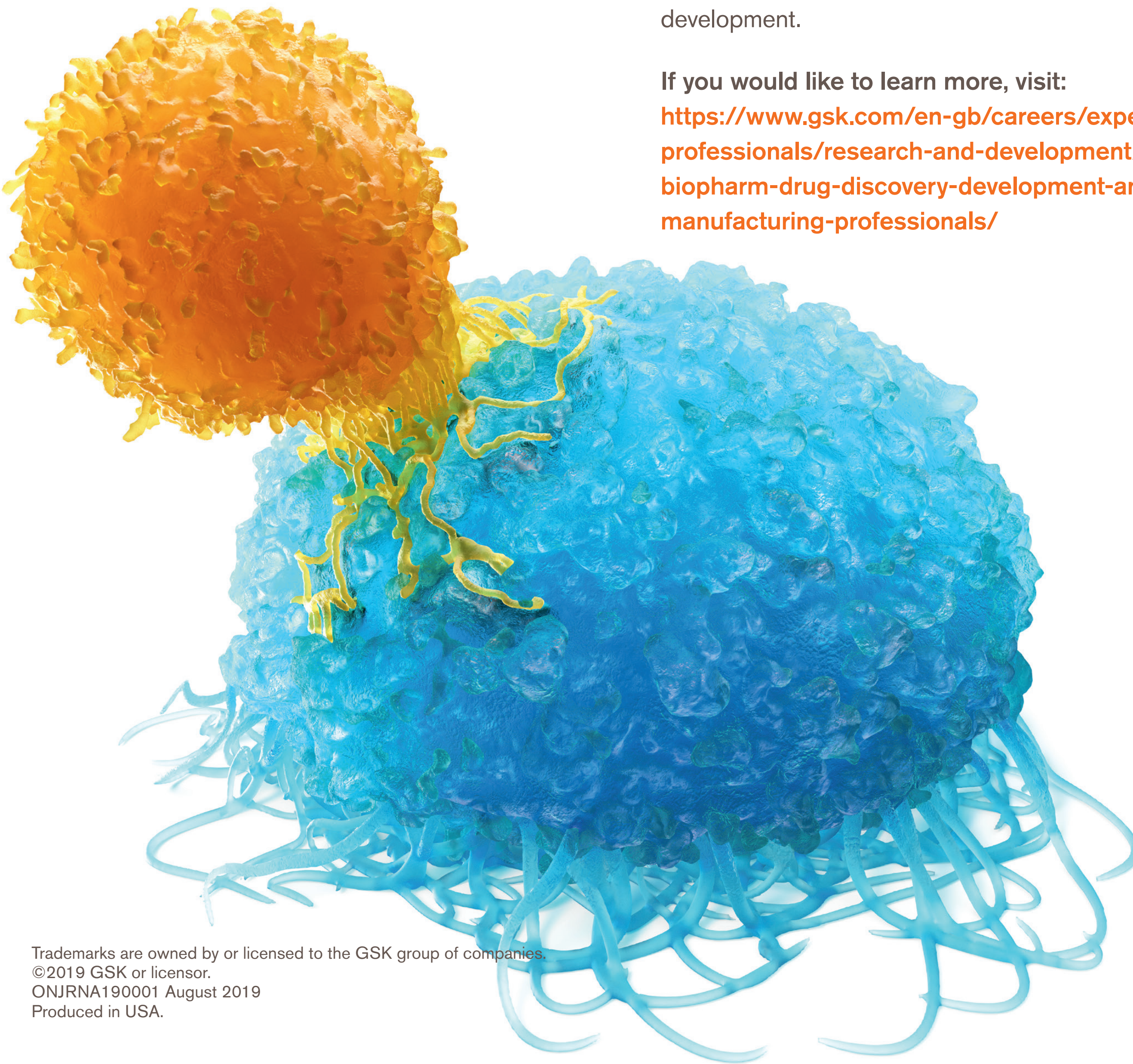


with a new looping algorithm, a new set of material parameters identified by research, and modifications to the mesh behavior.

With all this done, the image below indicates a perfect simulation in progress, with the ice detaching cleanly from the aluminum. No bending. No holes. No chipping. An almost perfect result.

As the simulation is perfected over time, it is no stretch to argue that we may shift from ice to more complex materials. Special thanks must be given to:

- Professor Raul Radovitzky
- Miss Zhiyi Wang (The graduate student behind most of the solutions and whose work I am reporting on)
- Miss Linsey Bjornstad (The graduate student who assisted in this project before me)



T-cell attacking cancer tumour

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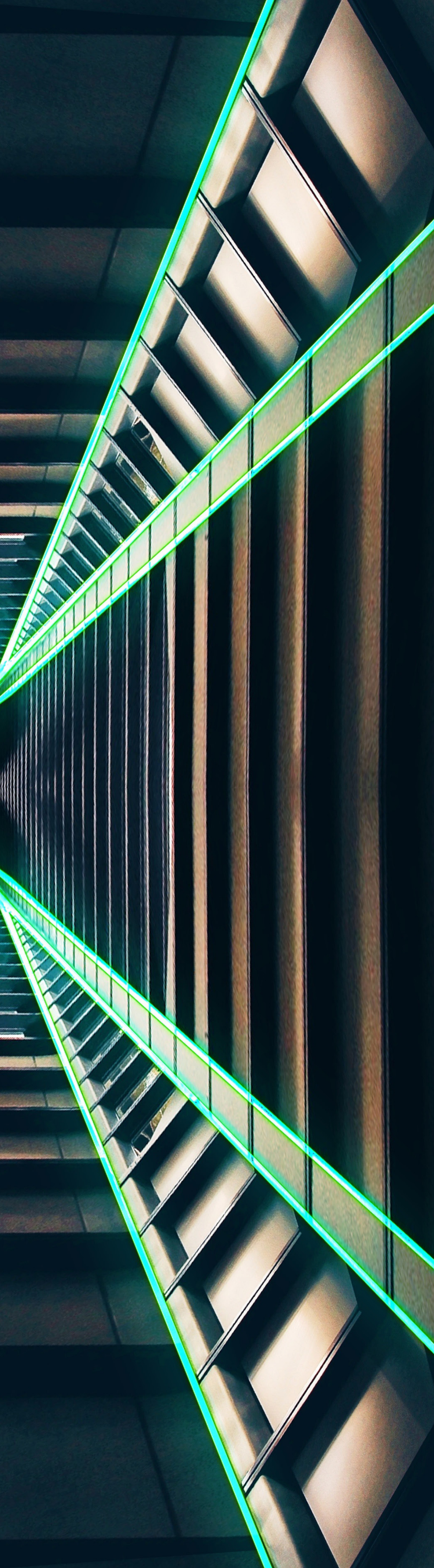
Community, Collaboration, Innovation

The Bayer Research and Innovation Center

Coming Soon to Kendall Square

Science for a **better life**



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MIT Undergraduate Research Journal

Massachusetts Institute of Technology

December 2021

Dear MIT Community,

As Fall 2021 comes to a close and IAP begins, we are delighted to present the 42nd issue of the MIT Undergraduate Research Journal. Throughout the past two years, we have taken part in countless experiences demonstrating the importance of community to science and of science to our communities. The MURJ team is proud and honored to continue in this spirit as we showcase the hard work, creativity, and innovation of our peers. This issue is published in honor of those who have sacrificed to protect their communities during this time. We are additionally grateful to the thousands of passionate and talented students across campus working to further knowledge in their fields, as well as the mentors that dedicate their time to training the next generation of researchers.

Enclosed you will find featured reporting on topics ranging from state-of-the-art quantum simulators, to AI-based heart failure therapy, to original commentary on the current state of life science research, to the study of ice fractures. Additionally highlighted are recent developments in MIT's outreach to high school students and the visions of Professor Gabriella Schlau-Cohen, who was recently recognized by the American Chemistry Society. Original student research published in this issue includes a biomimetic nanoplatform to aid the study of neurodegenerative diseases and a smart device and alternative compound to counter nicotine poisoning in real time.

As always, we acknowledge that the biannual publication of this journal is the product of hard work, collaboration, and commitment by MURJ staff members and often a product of years of hard work and investment by undergraduate researchers and their mentors. We would like to thank our editorial board and contributors for their time and hard work this semester and for persevering through the challenges of a largely remote school year. In addition, we would like to thank all the undergraduates who shared their research with us and the greater MIT community.

For previous issues of the MIT Undergraduate Research Journal, please visit our website at murj.mit.edu. If you are interested in contributing to future issues of the MIT Undergraduate Research Journal, we would be delighted to have you. Please contact murj-officers@mit.edu if you have any questions or comments.

Sincerely,

Gabrielle Kaili-May Liu
Editor-in-Chief

Massachusetts Institute of Technology

UNDERGRADUATE RESEARCH JOURNAL
Volume 42, Fall 2021

MURJ News

ARTIFICIAL INTELLIGENCE

Empallo: An AI Based MIT-spinoff to Watch

Innovators aim to create adapative heart failure therapy through artificial intelligence algorithms.

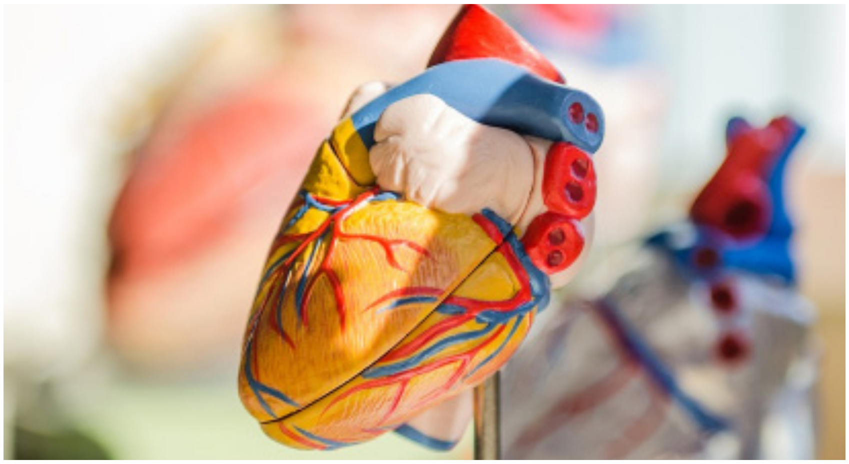
In September 2021, MIT's V Demo Day brought together budding university spun startups in culmination of the Martin Trust Center's delta V accelerator program. The teams showcased marketable innovations ranging from healthcare enrichment, to money transfer services, to social support platforms. Among the published list of 17 upcoming technological enterprises to watch is Empallo, a company started by Co-Founders Claire Beskin and Ray Liao. Beskin is currently an MBA candidate at MIT's Sloan School of Management who serves as Co-Managing Director of the university's $100K Entrepreneurship Competition, while Liao holds a PhD in Computer Science from MIT and works to develop machine learning methods and novel algorithms to apply to clinical problems. The company is additionally advised by Massachusetts General Hospital Cardiologist and EECS/Medical Engineering Sciences Professor at MIT, Dr. Collin Stultz, and has recently established partnerships with UCHealth, Mayo Clinic, and Beth Israel Deaconess Medical Center. But what does Empallo actually do?

"Half of all heart failure patients die within four years of diagnosis..." Liao contextualizes the complexity of long term heart failure treatment and remission in the United States during his delta V Demo Day talk. As he cites, 20% of heart failure patients are readmitted within a month of their discharge, and the US healthcare system spends $12 billion annually on heart failure hospitalization. Why is successful treatment of an increasingly prevalent disease (projected to increase by 46% by 2030!) so evasive?

"The fundamental challenge is the variability of this disease… When the patient is out of the hospital, the therapy has to be constantly adjusted for their dynamic and changing physiological state."

"The fundamental challenge is the variability of [heart failure] … the therapy has to be constantly adjusted."

The issues, Liao explains, is that heart failure therapies are not customized and responsive to individual patient needs after their discharge from the hospital. As such, standardized at-home treatment plans fail to elicit long term remission across broad patient demographics. Empallo aims to enable the creation of adaptive therapy via artificial intelligence algorithms trained on electronic health records and other biometric data. The goal is for the algorithm to learn post-discharge disease patterns, to ultimately be able to "…predict clinical trajectories and recommend timely interventions." The algorithm can specifically be applied to guiding discharge readiness, medication planning, and home monitoring.



With the expansion of digital record keeping in hospital systems, and growth projections for heart failure diagnoses, Empallo stands to make a lasting impact in the AI healthcare market. Liao and Beskin are currently working to market their service and establish new partnerships with integration health organizations and medical insurers. Learn more about Empallo at empallo.com

For a full list of "17 MIT startups to watch," check out: https://mitsloan.mit.edu/ideas-made-to-matter/17-mit-startups-to-watch.

— Prathysha Kothare

CHEMISTRY

The Award Winning Schlau-Cohen Chemistry Lab

Dr. Schlau-Cohen leads her team in cutting-edge biological and chemical research.

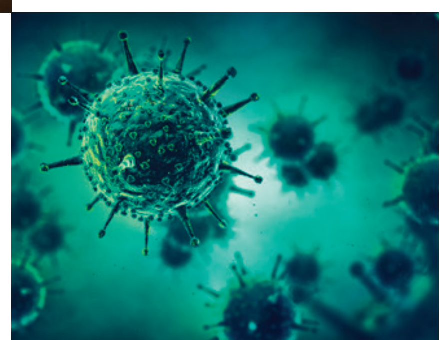
The American Chemistry Society annually recognizes the visionary and fundamental research of young individuals in North America through its Award in Pure Chemistry, and MIT's own Dr. Gabriela Schlau-Cohen has been named its 2022 recipient. With this recent distinction, Dr. Schlau-Cohen joins the ranks of brilliant researchers dating back 92 years to the award's inaugural winner and virtuoso of many trades, Linus Pauling. The prize is particularly dedicated to scientists with fewer than 10 years of experience since completion of their terminal degree, who have demonstrated "unusual merit" as well as "independence of thought and originality" in their chemical inquiries. So what exactly do Dr. Schlau-Cohen's seminal investigations concern? "… Lasers - Microscope - Proteins…" These lab website teasers are enough to elicit the curiosity of any scientific mind, and indeed the multidisciplinary research of Schlau-Cohen's team encompasses exciting applications across chemistry, optics, biology, and microscopy. She and her team of diverse graduate and post-doctoral students are particularly interested in applying the following methods, among others, to study biological light-harvesting and receptor protein systems, whose impacts range from improving solar energy technology to biomass production to medical therapeutics.

1) Ultrafast spectroscopy: Spectroscopy as a field concerns the characterization of spectra produced by matter or that which results from the interaction of matter with electromagnetic radiation. In this particular spectroscopic technique, an ultrashort pulse of light (with time durations on the order of 10^{-12} seconds) produces a broadband optical spectrum, and is used to study photo-induced events that operate on extremely short timescales. On a high level, these dynamics are captured by exciting medium with an ultrashort pulse, and thereafter probing it with a second light source to measure its absorption/emission profile over time. Several sub-methods exist within ultrafast spectroscopy, and Schlau-Cohen's lab has capitalized on these variations to describe energy flow, charge separation, and vibrational relaxation pathways that govern biological systems encompassing light harvest, chemical conversion, and membrane dynamics. Most recently, Schlau-Cohen's group developed a biohybrid photocatalyst to enhance the light harvesting capability and increase reactivity of photosynthetic systems under low energy irradiation! Read more about this work in their publication, "A biohybrid strategy for enabling photoredox catalysis with low-energy light."

2) Model membrane systems: Model membranes enable tractable investigations of specific properties and function of membrane components by isolating them in a physiologically representative yet simplified system. These membranes must be selectively engineered to express desired proteins, lipid composition, curvature, and stability. Nanodiscs are one such synthetic membrane system, and are composed of a phospholipid bilayer whose hydrophobic edges are screened by amphipathic proteins (i.e. membrane scaffolding proteins), peptides, or synthetic polymers. Nanodiscs offer high degrees of parametrization, ranging from lipid composition, disc diameter, surface area, disc stacking, etc. Schlau-Cohen's group employs these biological proxies to study membranous light-harvesting complexes and transmembrane receptors in vitro. The group simultaneously develops synthetic proteoliposomes with high membrane curvature and variable protein content to investigate higher order protein interactions. Just this year, the lab published findings that suggest the ability of membrane environments to tune the conformations and photophysics of light harvesting complex Photosystem II using fabricated nanodiscs and single molecule fluorescence characterization. Read more about the work, titled, "Membrane-dependent heterogeneity of LHCII characterized using single-molecule spectroscopy."

These projects exemplify but hardly do justice to the breadth, ingenuity, and ramifications of the Schlau-Cohen's lab research landscape. Since her appointment to MIT in 2015, Gabriella Schlau-Cohen has been bringing collaborative minds across STEM disciplines to branch into a vanguard of biological, energetic, and fundamental chemical inquiries. She will be presented the Award in Pure Chemistry at the ACS spring meeting in San Diego in March, 2022.

— Prathysha Kothare



MURJ Features

Arrange the Following Terms in Order of Importance:

Innovation, Funding, Applicability, Continuity

A brief commentary on the current state of affairs in the life science research ecosystem, narrated by its protagonists

By Arbri Kopliku

"And the most exciting part, even more than getting accepted to Nature Communications, is that it can get into clinical trials as early as next year," said Dr. Dan Goulet, postdoctoral research associate at the Koch Institute, during an informal interview this October. He was referring to his most recent co-authored paper on how IL-6 knockout mice exhibit a stronger immune response against acute lymphoblastic leukemia, and on how this finding can translate into curing human cancers.[1] As a curious but uninformed undergraduate I assumed that all great pieces of oncology research, much like this one, inherently contained a translational component that acted as the overarching motivation behind the project thesis in the first place. Seeing that my standards of evaluating research were slightly misled, Dr. Goulet went on to explain how the average shelf-life of research papers reaches almost a decade before they get dusted off and translated into the clinic. This sobering glimpse motivated me to better inform myself on the challenges that life science research at MIT faces on its path toward benefiting anyone besides the intellectual curiosity of the responsible scientist, and what determines its compatibility with the larger biomedical rebus of innovation. As I soon came to realize through my meetings with MIT professors and postdoctoral associates, it is all a matter of juggling time and attention between innovation in study approaches, procurement and retainment of funding, applicability of research outside the laboratory, and a guarantee that the project has a direction along which to keep growing.

My quest to better profile these components first led me to Dr. Bryan Bryson, Assistant Professor of Biological Engineering at MIT, whose lab studies everything there is to learn about tuberculosis pathogenesis and particularly engineering the host-pathogen interface as the infection is underway. His comprehensive answers very neatly fleshed out the research landscape that Dr. Goulet had sketched, despite studying as divergent ends of the human condition as offered by leukemia and tuberculosis. Funding is what allows ideas to turn into meaningful research, and according to Dr. Bryson it exerts undisputable influence on the paths chosen to address the more obscure parts of basic science. This unwelcome weight burdens the innovative approaches of the junior scientist much like it incentivizes the marginally incremental proposals of the senior one, thus propagating a complex interaction that reinforces itself upon ensuring the continuity of research work. While many Science, Technology and Society (STS) courses at MIT emphasize the deterministic role of innovation in motivating the natural course of research, funding turned out to be the most pragmatic lens through which to interpret Dr. Bryson's remarks, as well as to orient my following faculty interviews.

The biomedical research ecosystem conditions have to be exceptionally right for laboratory

1 https://www.nature.com/articles/s41467-021-26407-4

output to be taken up immediately by the field, said Associate Professor Michael Hemann of the Koch Institute, but there are lower-hanging fruits that scientists can aim at from the start of their experimental planning. Such is work in treatment protocols, where the individual drugs being studied have already been approved for safety and efficacy, as was the case with Dr. Goulet's group recommending the introduction of IL-6 antibody inhibitors earlier on in the ALL patients' drug regimens. Another potentially attractive field for fresh translatable research is that in diagnostics, and one in which Biological Engineering Professor Linda Griffith has extensive experience. She proudly summarized a good part of her research and advocacy career under the slogan "Endometriosis is not one disease," a strong argument in support of the importance that diagnostics holds in today's age of molecular characterization of disease. One of her many projects, a synthetic hydrogel, has seen an unprecedented spike in demand for use in human microenvironment modelling around the world, thus serving as a way of quantifying this gravitation towards diagnostics both in basic science and in engineering.

When it comes to funding, Professors Hemann and Griffith converged in their interpretations of where government funding for research currently goes: basic mechanisms are appreciated as the foundations holding the pyramid of progress in the field, but a hint towards future translatability is encouraged. One solution to this recurring obstacle, and one that rings closer to Dr. Bryson's own experience, involves coming up with research proposals that are daring enough to gain attention and consecutively funds even far from basic mechanism research. This risky approach has paid off in the past for Dr. Bryson, as his lab managed to pull money into tuberculosis work to develop the field's first CAR-T cells while competing with limelight oncology projects. The moonshot method is however quite unsustainable, as the gamble with such efforts by definition implies departing from the collective knowledge base and discontinuing that buildup of basic science expertise which could further delay applicable results in the statistically likely failure of the project. This is where the other biggest cash source in biomedical research comes in, the anonymous industry, which chases high risk – high reward opportunities to support undergoing projects from the successful proof of concept to the finish line, and that could sometimes get involved even earlier.

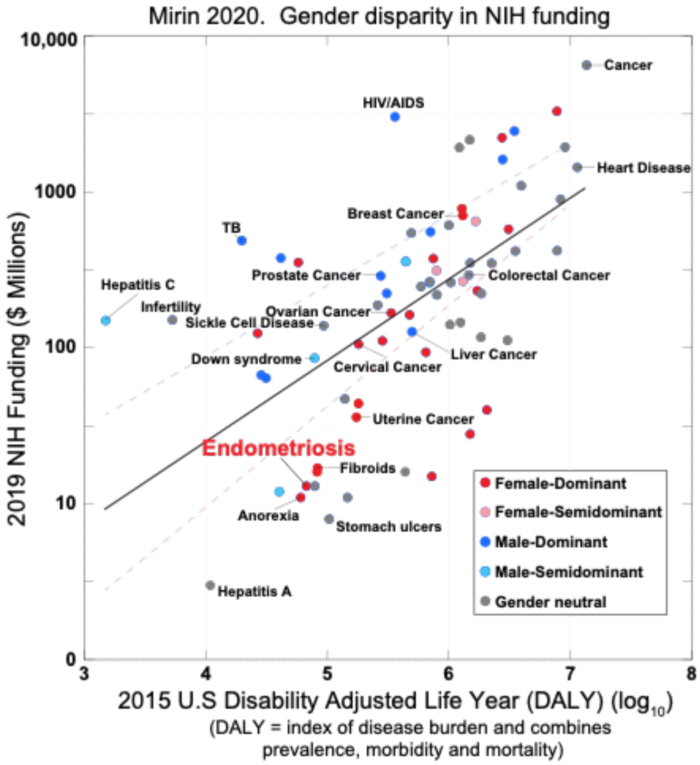
" Funding is what allows ideas to turn into meaningful research... it exerts undisputable influence on the paths chosen to address the more obscure parts of basic science."

Professor Hemann's following dichotomy of industry funding aligned with the image that each interviewee portrayed when collaborations outside the academic research space were brought up. The first mode of industry involvement consists of grants for "generically funded science," which allow researchers to pursue their interests while helping the companies explore different aspects of cutting-edge science that could be of industrial interest in the near future. An example scenario is Prof. Griffith's group working on c-Jun kinase while closely affiliated to Merck KGaA in Germany, a prominent pharmaceutical actor. Despite the legroom that this pocket of cash provides for out-of-the-box research, its unsustainability arises from the misalignment of scientific curiosities between the lab and the funding company, often because of the difficulties in making a product out of a selection of papers. In this case, Merck soon gave up on their c-Jun kinase pipeline and licensed it out to a smaller company, which also failed to carry the project over the regulatory phases. The second mode of this academia-industry nexus involves companies hiring research laboratories to solve ultra-specific problems of the field, much like contract research organizations. This option of ambiguous intellectual appeal provides even less reliability for continued research, in the unlikely case that such a perfect motivational alignment

Picture 1: *We do not readily associate MIT life with science expertise, yet the iconic Great Dome is less than 1 mile away from Kendall Square, the figurative downtown to the biotechnology capital of the world. This close relationship makes the state of the complex biomedical research ecosystem an incredibly relevant aspect of the future of the MIT campus and its contributions to the field.*

is found. Academic labs in general, and more so at MIT, have a reputation for being pricey both in time and capital thanks to their publication-bound scientific rigor, which makes most of these contracts short-termed.

One could interpret the outline of this article so far as an argument against moonshots, and they would be right to some extent. The knowledge buildup principle to which I alluded while analyzing government funding assumes the validity of existing literature, but such assumptions on the other hand can interact unpredictably with the surrogate targets of young innovative scientists. In other words, our biotechnological era of single-cell RNA sequencing and flow cytometry underscores a responsibility coupled with sufficient power in individual researchers'



Graph 1.1: Courtesy of Professor Linda Griffith, taken from "Gender Disparity in the Funding of Diseases by the U.S. National Institutes of Health" by Author Mirin, Ph.D. (2020)

hands to re-evaluate the status quo of their respective fields, and this obligation extends beyond basic mechanistic principles. An interesting and rather complex example is that of combination therapies for blood tumors, such as acute lymphocytic leukemia (ALL): many of them were developed empirically from the observations of prominent physicians like Sydney Farber, the namesake of the Dana-Farber Cancer Institute, and have remained mostly intact to this very day. According to Professor Hemann, it is even more challenging to raise funds for the kinds of research projects needed to explore the mechanics behind such empirical treatment decisions, and that stems from the industrial disinterest in bedside deconstruction of the standard of care. Instead, most of the support goes for the homerun quest, for single drugs that will individually cure complex diseases, while we continue to serve chemotherapy patients cocktails including many drugs of different toxicities, just because trial-and-error concluded so half a century ago.

This discussion of the biomedical innovation ecosystem would be incomplete without mentioning how research work can indirectly shape the cross-sector interactions within the ecosystem and outwards to attain a self-promoting character. An illustration of this would be Professor Griffith's endometriosis work, and also the reason why a renowned authority in the scientific sphere flies across the country on a regular basis to advocate for broader attention towards "gendered" diseases. She says it is her duty to the field to use her credibility as Director of the MIT Center for Gynepathology Research, and not just her research output, to inspire other researchers to take on similar issues and counterbalance the inclination of larger players such as the NIH towards genomics and artificial intelligence, at a time when discoveries in diseases mostly affecting women could readily translate into the clinic. Professor Griffith referenced Graph 1.1[2] to outline the disparities of NIH funding with regards to gender and disease burden, but it also goes to demonstrate the variety of priorities given to biomedical research areas in general.

Overall, the relationships between innovation, funding, applicability and continuity of research invite deeper scrutiny to expose the complex life science research challenges faced on a daily basis that overarch the ecosystem as a whole. My discussions with MIT faculty and research staff touched upon different perspectives on the connections between these four broad terms, and how they ultimately affect lives outside of the lab. Very diverse issues were raised throughout the interviews, ranging from the inconvenience of clinical trials to workplace credibility, though most of them could be categorized into the four above-mentioned boxes and were shared in both basic science and engineering settings. This piece was meant to act as a peek into the immense food for thought within the biomedical research interface to better educate the scientists of the present and policymakers of the future, but it by no means does justice to the full picture. I want to thank all contributors for their time and insights which gave a unique flavor to each argument, while shaping my own understanding of the current biomedical research picture characterizations.

2 https://www.liebertpub.com/doi/10.1089/jwh.2020.8682

Quantum Simulators that Solve the World's Hardest Problems

By Ezra Yaador

In a research collaboration between scientists from the MIT-Harvard Center for Ultracold Atoms and other universities, a new programmable quantum simulator with a record-setting 256 qubit storage was constructed recently, in the latter part of 2020. This development makes a significant jump from what has previously been achievable in quantum devices of its kind by several times, marking a huge advancement for humanity in the race for quantum computing. For some perspective, before then, the largest functional quantum computers developed by tech giants IBM and Google, world leaders in quantum computing, were 53 and 54 qubits in size, respectively (5, 6).

"The hope is that there is something exponentially better or, at least, stronger than a classical computer."

For some background, qubits (quantum bits) are the classical computer bit ("0's" and "1's") analogs of quantum computers. However, instead of just taking on one "0" or "1" state at a time, qubits can be in a quantum mechanical superposition of those two states, or a "0" and "1" at the same time. A system of x qubits would yield 2^x complex coefficients or amplitudes, equivalent to quantum storage units. Therefore, while a system of 500 bits would yield 500 storage units, a system of 500 qubits would yield more storage than atoms in the universe (7). Because of the vastness of such quantum systems, quantum-based algorithms are suspected to be able to operate at speeds impossible for even the fastest supercomputers. Qubits are derived from various types of quantum particles and structures, such as trapped ions, photons, and optical lattices.

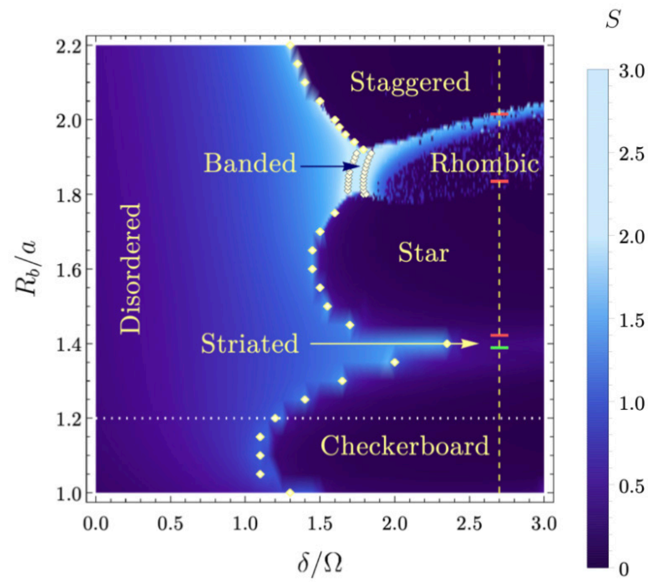
Quantum simulators are a special type of quantum computer that utilize, for example, laser-cooled neutral atoms (with superimposed atomic "spin up" and "spin down" states serving as the "0" and "1") to solve physics problems at the atomic scale. The applications of these simulators are more limited than universal quantum computers as computers are theoretically meant to do a variety of calculations, including those outside of physics. However, quantum simulators can prove to be superior as they can solve many major scientific problems that quantum computers, due to their lack of well-controlled, error-corrected qubits of sufficient quantum volume, are decades away from solving (2). Therefore, quantum simulators, rather than all-purpose quantum computers, may serve to provide the "quantum killer app" that many have been seeking to facilitate humanity's advancement into a world of quantum technology. As a result, QuEra, a quantum computing startup founded by the researchers that is launching accessible versions of their simulator by 2021, has already raised $17 million from investors, including Tokyo-based e-commerce company Rakuten, and generated $11 million in revenue (4).

In an earlier collaboration in 2017 that included Professor Vladan Vuletić, a co-developer of the new simulator and co-founder of QuEra, the team constructed their original version of the device with a storage exceeding that typically produced at the time: 51 qubits. They utilized ideas known at the time but believed not to work very well, but according to Professor Vuletić, the entire process worked magically well.

"So before, people could already trap individual atoms into individual traps, but only with about 50% probability. That made it so that if you have a large system of 10 or 20 or 50 traps, you would hardly ever exponentially fuel instances where you trap all of the atoms." However, Vuletić and his team discovered that, after randomly loading atoms into the array, one can look at which array positions on the 2D quantum simulator are filled with multiple atoms and, from that, redistribute those atoms to quasi-deterministically load one atom per trap. "It's really this trick at the moment that works rather well."

However, in this latest discovery, the scientists utilized a more efficient protocol which enabled them to move entire rows of atoms in parallel with two sets of movable optical tweezers, or lasers. Multiple moving traps aligned in parallel enabled multiple atoms to be moved up their respective columns at once, creating the much larger 2D arrangement of atoms. As stated in their paper, the entire process only takes 50-100 milliseconds with more than 99% of the array filled.

In their paper, the researchers used the device to study quantum phases of matter: a star phase, a striated phase, and a checkerboard phase. These phases arise from the atoms adopting lowest energy conformations in the array when their interactions are increased to certain strengths, analogous to, for example, liquids conforming to solid crystals at certain temperatures and



Quantum phase diagram with phases studied by the simulator from a previous paper. The axes represent parameters for the atoms' interaction strengths. At certain interaction strengths, the atoms transition from disorder to the various phases. Used with permission from (7).

pressures. However, the atoms' behavior in some phases, such as the striated phase, cannot be explained by just classical particle, or crystal, dense-packing; their 2D alignment arises, in part, from quantum fluctuations. In between the phases, the scientists were able to observe quantum phase transitions for the first time ever, specifically in the Ising (2+1) dimension (2D plus time dimension) universality class. The Ising Model serves as the benchmark model system for studying phase transitions in both classical and quantum matter; it's essentially the Drosophila fruit fly of physicists (3). Therefore, with their discoveries, the researchers made significant contributions to studies of quantum many-body

"Already, the simulator has allowed researchers to observe several exotic quantum states of matter that had never before been realized experimentally, and to perform a quantum phase transition study so precise that it serves as the textbook example of how magnetism works at the quantum level." -The Harvard Gazette

behavior that have implications for quantum material and device optimization.

A significant feature of the simulator is that it can be used to conduct fundamental research and directly study quantum phenomena in all types of processes. For example, in chemistry, the device can directly emulate molecules and chemical reactions, and it can even determine whether the products of a reaction can be modified just by manipulating the wave functions (particle-wave duality) of the same starting materials. In biology, the simulator will be able to reveal the role of quantum effects in photosynthesis. In general relativity and cosmology, the simulator can be used to study various theoretical phenomena, such as quantum effects in curved spacetime, by simulating them, and when combined with high-precision measurements, it can even be used to detect and study gravitational effects. In quantum transport, it can create and simulate quantum complex networks, including models of a future quantum internet.

According to Professor Vuletić, elucidating the scaling behavior of certain quantum studies and computations were one of the main motivations for the quantum simulator expansion.

"Quantum computers, as they work right now, won't be better than classical computers, but we're interested right now in how they scale," he says. Studying scaling behavior would shed new light on how fast quantum computers can do certain calculations, and it would show how much advantage qubits have over classical bits as a computation becomes very large.

"The hope is that there is something exponentially better or, at least, stronger than a classical computer."

One of the biggest challenges moving forward in designing quantum computers, he says, is in their storage encoding.

"In a classical computer, we encode bits redundantly, meaning we make several copies of the same memory bit, and if one of them gets lost because, you know, a high energy particle flies through your computer, you still have the other copies and can correct any errors that happen."

However, in quantum computers, this is much harder to do. Merely looking at the state of a quantum bit, for example, would actually destroy a part of it (due to quantum decoherence); instead, one would have to compare pairs of qubits and, from that, derive their states. The analogous method of error correction in quantum computers, termed Quantum Error Correction, has been theoretically proven to work, but no one has fully demonstrated it in a quantum computer yet.

"With the current schemes, we would need many, many quantum bits to encode just one logical, protected quantum error code."

With a developed protocol for quantum error correction, the researchers, along with others, will eventually be able to develop universal quantum computers of larger scale that can solve the world's outstanding scientific problems. However, quantum simulators are taking on that role right now, and they, actually, may be the quantum devices that facilitate humanity's advancement into a world of quantum supremacy.

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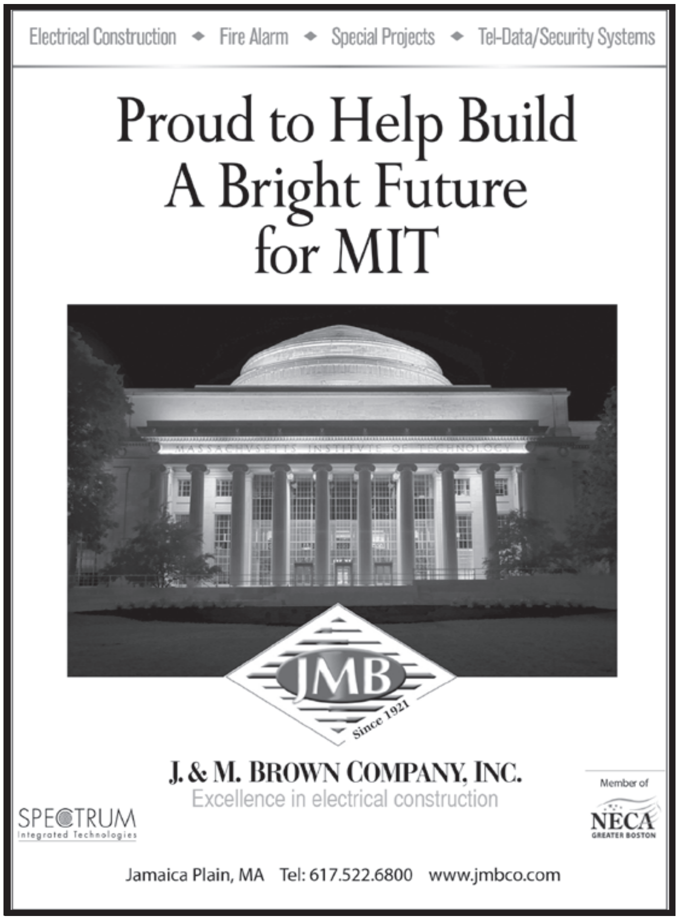
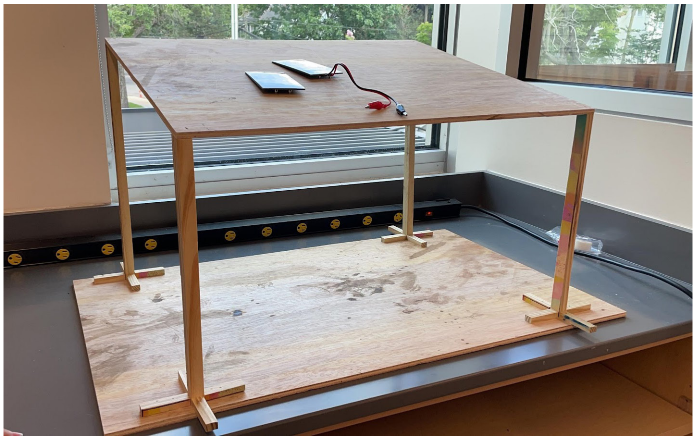


An Exciting Outreach Opportunity: Expanding MIT's Connectiveness with High Schools

This issue's spotlight features Ed Moriarty and Chris Mayer

By Lia Bu

Before Mr. Ed Moriarty, an instructor at MIT's Edgerton Center, concluded his mini building workshop offered to accepted students during the CP* week, he offered an interesting opportunity to those in the Zoom call. To those interested, he and Mr. Chris Mayer, the clubs and teams liaison, proposed an idea that revitalized and expanded the impact Global Teaching Labs (GTL) have on their students. Due to COVID-19, the limited travel impacted this program. Therefore, Mr. Ed Moriarty's alternative solution included accepted students to MIT (and therefore incoming first years) could develop and run an engineering design workshop (EDW) program that allowed the first-year's high schools and the Edgerton Center to connect and explore teamwork and design projects. Out of the 20 or so in the first Zoom call, the collaboration solidified to include Victoria Velazquez, Grace Jau, Catherine Tang, Abitha Vegi, Yitian Zhu, Sarah Lu, and myself (Lia Bu). Out of 6 people, there were four high schools that participated in this program: Seven Lakes High School (Katy TX); Mission San Jose High School (Fremont, CA); Hialeah Gardens High School (Hialeah Gardens, FL), Woodside High School (Woodside, CA), and Isidore Newman School (New Orleans, LA). Each of the four teams developed a team or teams of students that led projects ranging from 3-4 weeks of the program. To encourage collaboration, all the schools began with a fun activity: launching water rockets! This activity encouraged a team-working dynamic that served well when the main projects ideation



The Initial Stand

process rolled around in the second week of the program. Each team additionally had sophomore mentors in addition to the rising first years connecting back to the Edgerton Center and MIT's resources.

Developing this project at my high school (Isidore Newman) included many different moving parts. In April and May, I attended weekly meetings that allowed first-year students and me (named FRED) to develop this program, and to build leadership skills. Within my school, I worked with Mr. Matthew Jones, the head of the science department, and Dr. Andrew Hermann, the chemistry teacher. We all were very excited to see how the program would turn out, and began the program around a week early to meet with the team and begin to generate ideas for potential projects.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In our first meeting (after the team-building rockets), both Mr. Moriarty and Mr. Mayer wanted to encourage crazy team building ideas, even if they weren't feasible. The four students participating in the program scampered around the room, writing down random ideas on sticky notes and organizing them on the white board. My personal favorites included a painting soundscape, which could transform images into sounds, a solar-powered car and stove, a Stirling engine generator, a smart bike stand, and an interactive game. These ideas were taken apart, smushed together, and completely transformed in a way I didn't think was possible. Watching the team interact in generating these ideas using their imaginations and creativity was amazing and demonstrated that teamwork is crucial in any design process, as the best ideas from my team came from throwing around random concepts.

As a result of this two-day ideation process resulted in two main projects that were pursued, along with individual work. The side project that two out of the four team members pursued included building a 3-D game of clue. Building upon an original CLUE Board, they envisioned building a house on top of the foldout and making it so that the piece travelled in a three-dimensional space, adding to the complexity of the game. Using both CAD modeling and hand-drawn plans, they truly improved on the game, even by changing some of the rules to make it fairer. Unfortunately, the laser cutter was unable to be used until the beginning of the school year, but the foundation of the project was completed successfully.

The big project that all four team members pursued came from a mash-up of the "smart bike stand" and the "solar-powered car." The team thought, "why not put them together?" Therefore, the team quickly began to pursue a solar-powered charging station for e-bikes, that would sit on Isidore Newman grounds able to be used by any member of the community that commuted with e-bikes to school.

Since this was such an expansive project (as we were building it from the ground up, no pun intended), there were initial doubts on its feasibility. However, I believe that my team was particularly suited to this project. Each of the four members was knowledgeable of a certain part of the project. For example, one handled electronics, as he was very invested in batteries, currents, and wiring. Another handled the design and the modeling of the structure, as he was experienced in CAD modeling and design. The other two members wanted to learn more about woodworking and the construction of the project, and so they contributed significantly, along with the others, to making the physical prototype and the building of the physical structure. All three different fields played off of each other very well, creating this hub of designing, pushing ideas, and innovative solutions to problems that we ran along into the way.

During the beginning of the thinking of this project, the team did research, calculations, and compilation of the materials that might be necessary. We first began with a prototype of the stand. The prototype initially consisted of a

The Building of the Structure

rectangle platform laying on 4 legs (like a table) but was slanted around 15 degrees (so that one pair of legs was lower than the other). On this slant, the solar panels would lay to catch the solar rays. We had not thought of where the box holding the necessary electronics would go, and we did indeed run into this situation later in the main building process. To support the legs, there was cross bracing on the bottom, acting as feet.

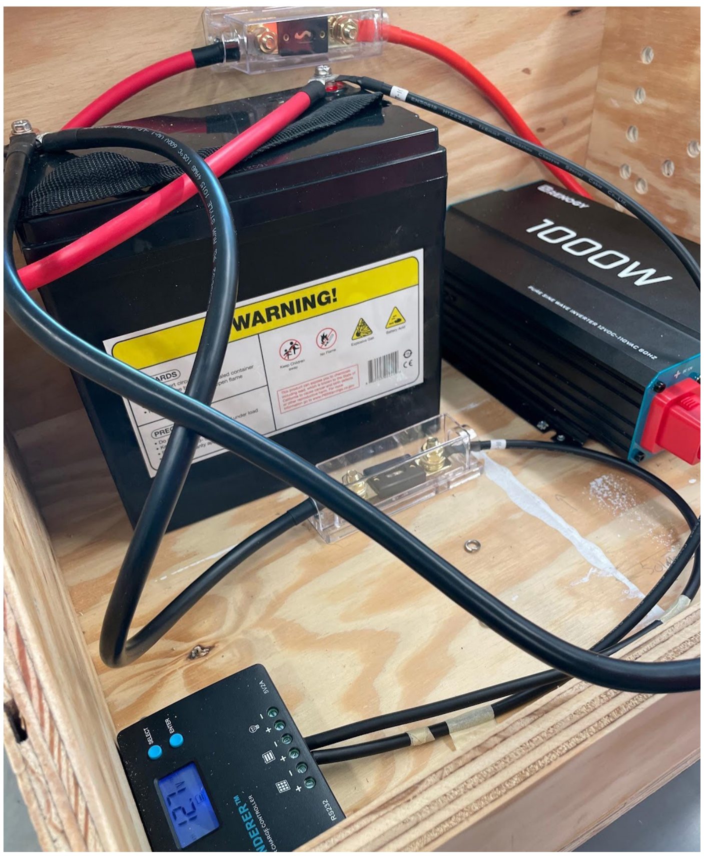
> *"The big project that all four team members pursued came from a mash-up of the 'smart bike stand' and the 'solar-powered car.'"*

When the team proposed the idea to Mr. Moriarty and Mr. Mayer, it was clear that there were critical design challenges in the proposed build. Firstly, the 15 degrees were not sufficient to catch all of the rays possible, missing out on the maximization of the solar charge. Based off the latitude of New Orleans, the roof of the panels needed be 30 degrees slanted. Secondly, to make this a sound structure, the design needed cross bracing not on the feet of the structure, but on the legs (making an X across the smaller and longer legs). We additionally would need extra 2 by 4's to stabilize the roof, so that it could hold up the solar panels. The team designed this structure in mind to withstand very strong winds New Orleans, and so the design needed to be completely stable. Our sophomore mentor, Charles Bales, is an architecture major, and so he made very insightful comments to improve the build.

A critical member of this team not originally part of the project was the school's Technical Theater Director, Mr. Philip Cramer. Without his knowledge and guidance of construction, the project would not have been possible. He additionally provided comments that were additionally helpful, as he was there in person watching the construction and providing real-time feedback.

The team went back to the drawing board, but additionally, during this time, the electronics required also began to be drafted. Because I was

purchasing the necessary materials, I worked closely with Mr. Jones and the team member focusing on electronics. We eventually settled on a system that greatly eased any unnecessary work required on the circuitry and made it safe: we purchased mostly Renogy products. This eased the circuitry, as we did not have to spend time figuring out if different devices from different companies were compatible with each other. However, we did have to buy the wires separately due to shipping delays. We did unfortunately run into the zone of waiting for materials, but this was remedied by watching science videos and pursuing quick projects, such as the construction of a model airplane and expanding on the 3D-clue project.



The wiring of the electronics box

However, once the supplies all arrived, it was crunch time! The team originally met for four hours each day during the weekday, but this sometimes stretch to five hours as there was a lot to accomplish. The team started by constructing the main frame of the build. Cutting around seven and nine feet of 2 by 4's was challenging, but with Mr. Cramer's and Dr. Hermann's directive, the team accomplished the main frame in around 3 days. This included using carriage bolts for the frame, which theoretically would allow for quick dismantling of the structure in case there was a hurricane about to land. This wasn't the case, however, and the structure was so large and heavy that it was very hard to put up and take down and put up again. Therefore, we no longer worried about truly taking it apart after it was built for the last time. All four contributed to painting the primer on the wood and letting it dry. Around this time, we ran into the technical challenge of storing the electronics safely.

The biggest concern about the electronics (which included a solar charge controller, a battery, and an inverter) was storing it safely. Outside, the electronics would be subject to the elements and any critters it might encounter. While our first idea was to place a weatherproof box in the corner, the team quickly realized that the electronics were quick to get hot, and that they ran a chance of overheating in a closed box. However, placing mesh on the box was extremely difficult, as the box was designed to hold only the electronics, minimizing as much space as possible. As a result, the team bolted it to the underside of the roof. This was extremely successful (although difficult, as the box weighed around 40 pounds)! For the circulation of air, we drilled holes in shape of an N for Newman and painted in green, so that it was visible to those that used the bike station or passed by it.

When we were finally ready to build it outside (as it was so large it couldn't fit through the doors or on the truck) the team enlisted the help of their parents. Their parents dropped by at one time or another, one of them bringing supplies for the project with her. Another helped us lift the massive 2 by 4's and the ten feet by four feet roof onto the platforms. At times, it was excruciating to work in the 95-degree heat, with the sun barreling down as we worked in the afternoon (we had to then move it to earlier in the day to finish the project). I could feel the camaraderie in the air as we worked to finish the project with both the team members and their families.

We spent the next few days painting it, hooking up the solar panels, and wiring the circuitry together. A team member additionally added further artistic details to the frame. He painted green stripes down the cross-bracing, adding a nice pop of color to the frame. (The green and white refer to Isidore Newman's school colors). As a result, it fit in perfectly with the theme of the school and its location next to the football field. An added benefit of the project the team thought of included its use when not as a bike stand. During games, it could serve as cover for the ticket stands and would allow people to charge their phones or other devices off the solar power.

With the succession of the project, the last final push for the team was to compile all their work for the month and create a presentation. During this time, we were able to hear about the projects from the other schools as well. For example, from California, my team heard about how it was like to design unique games, and their experiences with the bottle rockets. When it came time for Newman to present, my team did it smoothly. Detailing both their challenges and success that led to the completion of the project, some of the biggest takeaways for the team members included exploring working on a team well with a big project, learning about different types of engineering, and being exposed to the building and woodworking process. Both Mr. Moriarty and Mr. Mayer were proud of the work, as was I, for the work and learning the Newman team did throughout the summer. The team was able to break down an idea that seemed overwhelming into an extremely successful project that charged a computer, a power tool, and is currently used by the faculty at Newman who utilize e-bikes.

As for myself, I learned during the summer how to lead a team of different personalities, interests, and experiences towards a common goal. Interacting on problems has helped me transition to MIT, and the collaboration I did with my fellow classmates and the Edgerton Center gave me a change to adjust quickly to my first year at MIT. Regarding my team, I offered advice when I could, compiled information, and proposed solutions. However, this project was truly team-drive by the high schoolers, and it was phenomenal to see not only the project's growth, but their growth as well in learning how to think, problem solve, and use their imaginations. Reflecting on the program, starting from a CAD design model to an actual structure that currently stands tall at Isidore Newman School seems mind-boggling. However, with the help of Dr. Hermann, Mr. Cramer, Mr. Jones, Mr. Moriarty, and Mr. Mayer, and Charles, my team worked very effectively for four weeks and were able to produce a project and a program they and Newman can be very proud of. I cannot wait to hear about what they do in the future as they continue to grow and use the skills learned in the program.

Cracking a Path Forward: Ice in the World of Fracture Simulation

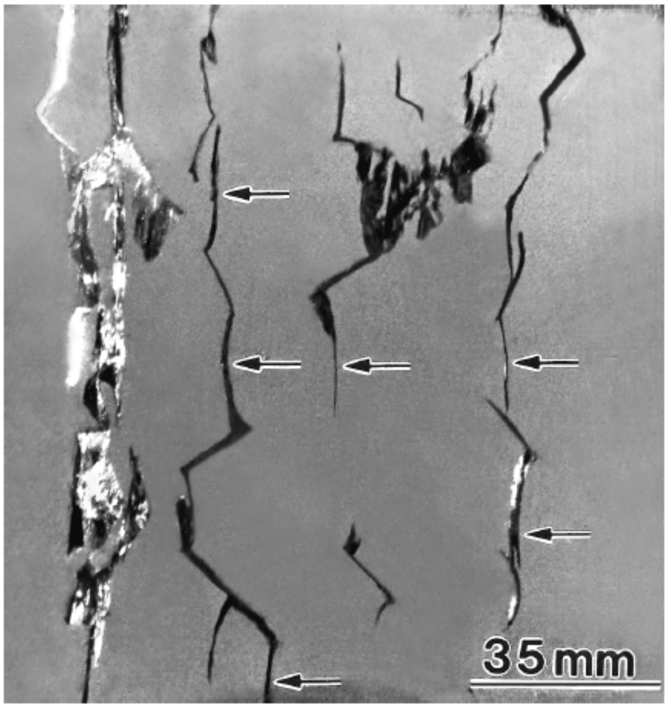
By Hillel Dei

"We cannot ignore the vital role of ice in the ecological system, in the polar caps, and in moderating the global climate"

Ice. You know what it is. I know what it is. You've played with it, used it to freshen up your beverages, used it to soothe injuries, and may even now be doing something with it as you read this article. You might even be listening to, "Ice, Ice, Baby." Then, we cannot ignore its vital role in the ecological system, in the polar caps, moderating the global climate. But here's one thing I bet you'd never have considered. Have you ever looked at ice and thought: Hey, let's use this as the basis of a new modelling system? Have you ever watched your ice fracture, and then imagined setting up a series of experiments in collaboration with the United States Government to try to anticipate how cracks propagate within ice, and use this as a building block to anticipate how cracks behave in general? I'm guessing you, oh reader mine, did not yet imagine having done that. Allow me, to introduce to you, the wonderful world of fracture simulation.

Let's begin by turning back the clock to provide some historical context. From 1944 to 1961, the research agencies known as the Frost Effects Laboratory, SIPRE (Snow, Ice and Permafrost Research Establishment), Arctic Construction and Frost Effects Laboratory (ACFEL) were established. This subdivision of the U.S. Army Corps of Engineers conducted research, as I am sure you can imagine, around ice and frost: from means of construction in cold regions to how best to transmit signals in this extreme terrain. From the chemistry within soil in extreme terrain to tracking water bodies. Anything ice-related was done by these groups, which has evolved over the years into the organization currently known as CRREL (Cold Regions Research and Engineering Laboratory) and still a close affiliate of the US Army. With this historical context in mind, we may appreciate how a collaboration was struck between the fine engineers of MIT and the snowmen of CRREL, with both being highly research-intensive organizations and CRREL's projects easily aligning with MIT's mission toward the betterment of mankind.

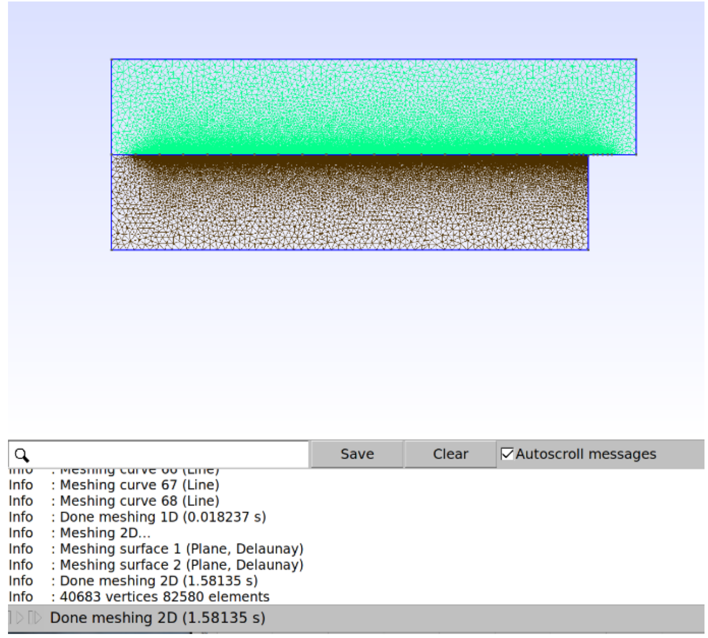
The phenomenon of ice cracking had long been a well known one. I mean gosh, just chew on ice picks and you'd easily observe it. It was also understood that the unique nature of ice—which permits easy identification of cracks, simple control of experimental errors through increased trials, elastic behavior that obeys Hooke's law over a reasonably large area (meaning plots of its load-displacement curve would be reasonably consistent), and remarkable cohesion while cracking—makes it the ideal candidate. In this context, an experimental plan was put forth, and MIT's partners at CRREL decided to conduct the following experiment: a sheet of ice, bound to a thin slab of aluminum as illustrated below, would have some force applied to it. This would induce a shearing effect and a plottable load displacement graph that could easily adopted for modeling. In other words, this would give us a reasonable goal and a specific target to work toward: an experimental value to chase, if you will.



Source: E.M. Schulson; The fracture of water ice: A short review

Now comes the fun. With the experimental results in hand, we were tasked with creating a simulation of the ice fracture. Allow me to put this in context. MIT, or more specifically the Radovitzky Research Group, was tasked with creating a software simulation of the ice fracturing experiment that reproduced, or came reasonably close to reproducing, the physical cracks induced.

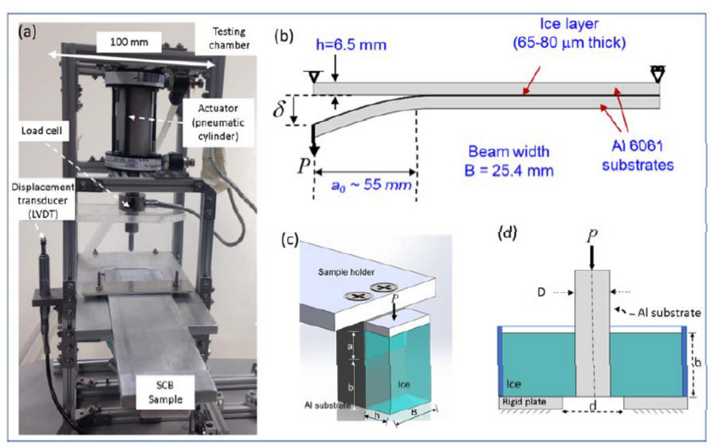
To provide a massively oversimplified explanation of the tools used in simulation: MIT researchers constructed a software package in which a facsimile of the structure of ice was constructed using a triangular mesh (an example of the generation process is given in the image to the right above). The size of this mesh could be altered to increase or decrease the number of triangles within it. The program functioned by performing calculations at each time-step, such that the parameters used in calculation could be modified. Thus, other possible alterations included changes to typical material properties like Griffith Energy, elastic modulus, and Young's Modulus, among others. This variety allowed for significant versatility in simulating the behavior of ice: simulations could be run repeatedly with alterations to the mesh and material properties, in order to achieve a closer match with the



Example of the mesh generation process

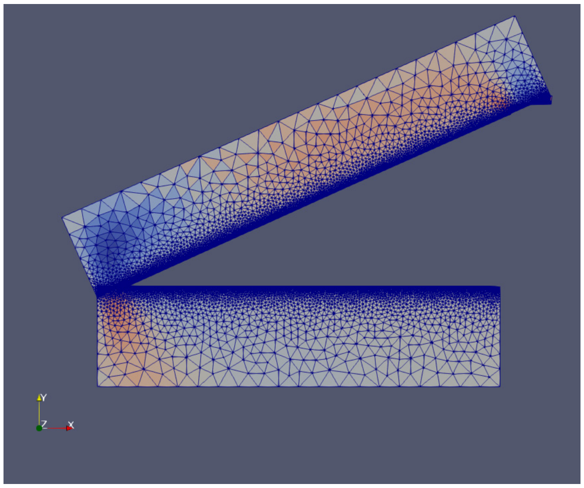
experimental properties observed.

Given this setup, the software could permit a crack to propagate: the load and energy travelled along the ice-aluminum boundary with the result of each successive stage based on the outcome of the previous time step until the energy had been sufficiently dissipated, or until the crack had fully propagated and the two materials were separated. For confidentiality, I cannot divulge the actual models used. However, the publicly available experimental results shown below will serve just as well to help us visualize the experiment performed, and the results we sought to approximate:



Source: Dawood; Characterization of Ice Adhesion: Approaches and Modes of Loading

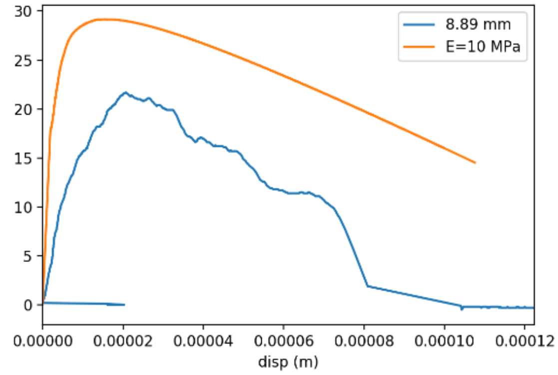
Depicted below is an example simulation of the ice fracture experiment. To learn more about the specifics of the math involved, and how the simulation kit was created, please refer to the following paper by Professor Raul Radovitzky: "A scalable 3D fracture and fragmentation algorithm based on a hybrid, discontinuous, Galerkin, cohesive element method."



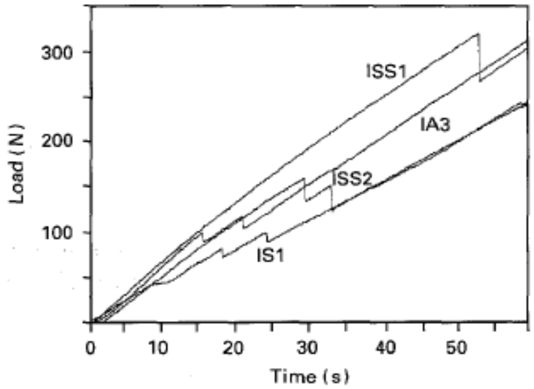
With the aforementioned goal in mind, let us now proceed to examine the extraordinary progress made in this research; this is easiest done by comparing the simulated load-displacement curves with the experimental results obtained. After months of improvement, our results came extremely close to the experimental observations, and this was no easy task.

In addition to the following graphs, the first image on the subsequent page effectively summarizes the essence of this project: at each time-step, based on the methodologies used by Radovitzky et al., calculations were iteratively performed to determine from the results of previous time-steps the load and then the displacement. This permitted creation of a model of how the crack propagates. Parameters were pulled from a material data file for simulations.

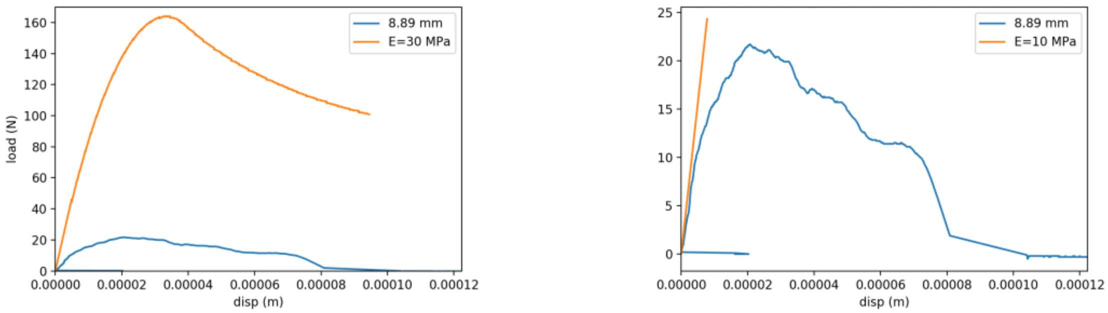
In my experience, the single greatest problem we faced, and one of the earliest problems, in fact, was the violation of the constitutiveness



Depiction of one of the more recent load-displacement curves, with the blue line representing the experimentally derived trajectory and the orange line representing the theoretical trajectory.

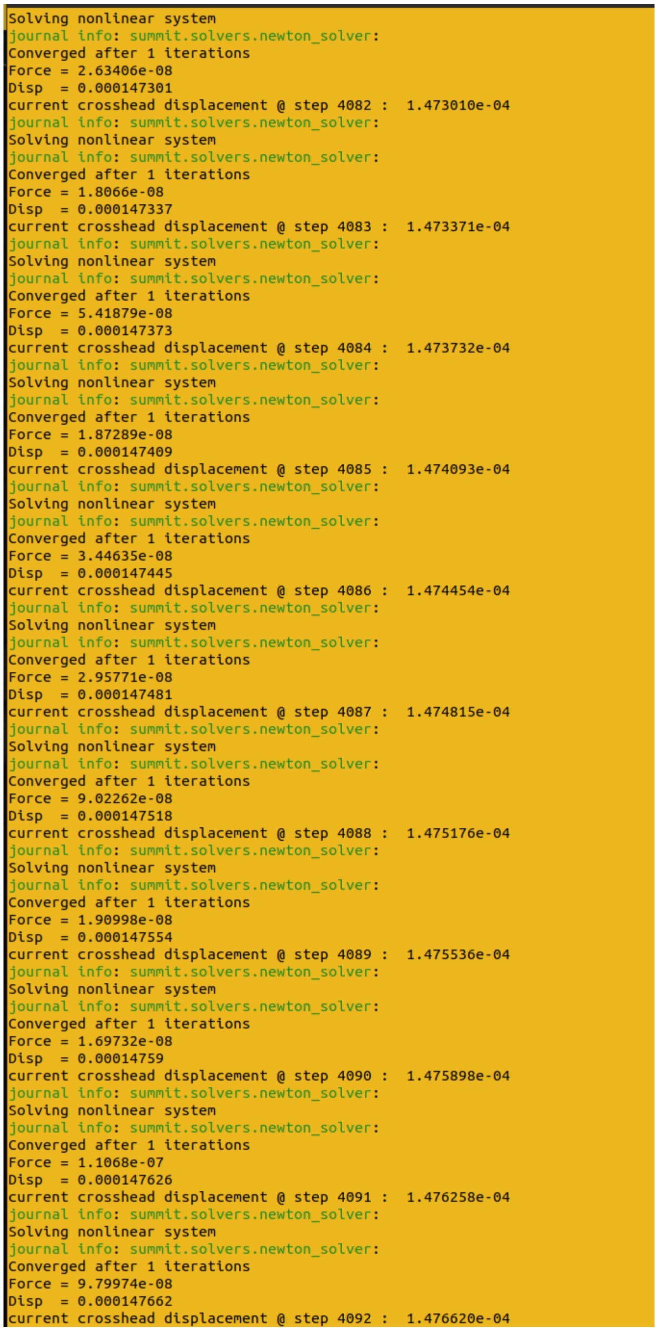


Example of a typical load-time curve as opposed to load displacement, again used in lieu of confidential results. Source: Y. Wei; Ice/metal interfaces: fracture energy and fractography



E=30 MPa E=10 MPa

Depiction of the extent to which varying the material parameters can affect the results yielded by the simulation kit



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Solving nonlinear system
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Converged after 1 iterations
Force = 2.63406e-08
Disp  = 0.000147301
current crosshead displacement @ step 4082 :  1.473010e-04
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Solving nonlinear system
journal info: summit.solvers.newton_solver:
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Converged after 1 iterations
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Converged after 1 iterations
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Disp  = 0.000147662
current crosshead displacement @ step 4092 :  1.476620e-04
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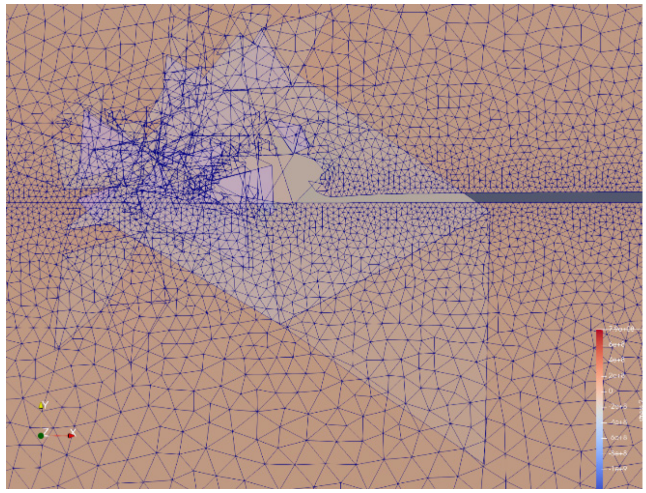
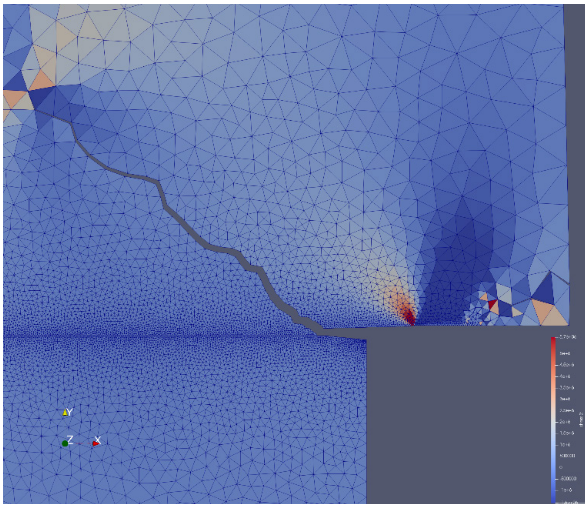
property. In simple terms, this property means we cannot have two entities existing in the same spot at once. We unfortunately ended up with this exact problem, indicating that our results needed fixing. The image to the right above depicts a sample mesh output by our simulation kit for which the constitutiveness principle is clearly violated. To address this problem, we utilized a redesigned mesh in which the triangle looping path was altered and a three-layer mesh was created. As there would be an extremely thin layer of aluminum oxide between the ice and aluminum, this intermediate layer could act as a buffer against more extreme conditions.



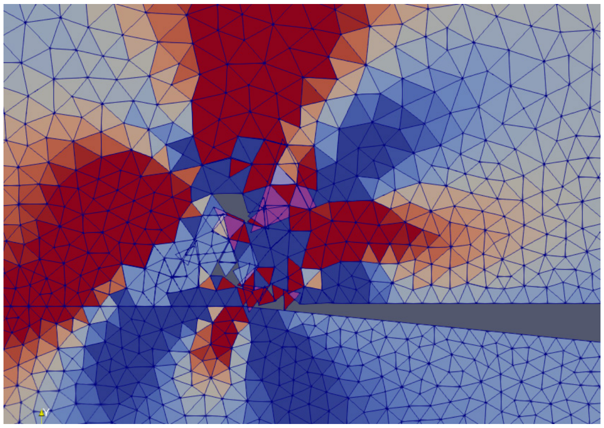
The next failure case encountered was mesh disintegration. To provide an illustration of this: please consider the difference between ice and snow. If you were to take a blade and cut through ice quickly, it would split into 2 pieces while still retaining its shape. Contrast this with snow, for which the same procedure would cause an almost explosive effect in which the snow falls apart. Intuition predicts that ice would not behave in this manner. Yet according to the results of our mesh, this was indeed the case. To resolve this issue, careful adjustment of the aforementioned material parameters was required.

Following this challenge was a case of inconsistent elastic behavior. To provide a bit of intuition from the real world, allow let me ask a simple question. Have you ever seen ice bend? No? Me neither. The results of our simulation seemed to differ, and resolution of this error required research into acceptable material parameters which we could justifiably claim to use in our simulation, along with a reworking of the mesh loop, which eventually was, too, resolved.

To explain the third challenge encountered, it is easiest to explain the solution first. Increasing the interface energy made it more difficult for the crack to propagate into the ice itself and not along the boundary. In other words, the crack was expected to move along the interface between the ice and aluminum, but curiously it propagated into the ice, as shown below. To solve this, we increased the interface energy until there was no way a crack induced by force of that order could penetrate into the ice, and when the latter issue resurfaced at a subsequent time, it was easily addressed by the three-layer mesh, since the aluminum oxide layer between the ice and aluminum was uniquely set up to prevent the crack from breaking into the ice.



The final challenge encountered was the curious case of chipping, depicted below. Effectively, holes were being created within the mesh as the crack propagated, and this was more of an amalgamation of prior problems: the crack's propagation into the mesh and the mesh's own failure to remain intact. As such, the solution to this problem was the sum of all prior solutions,



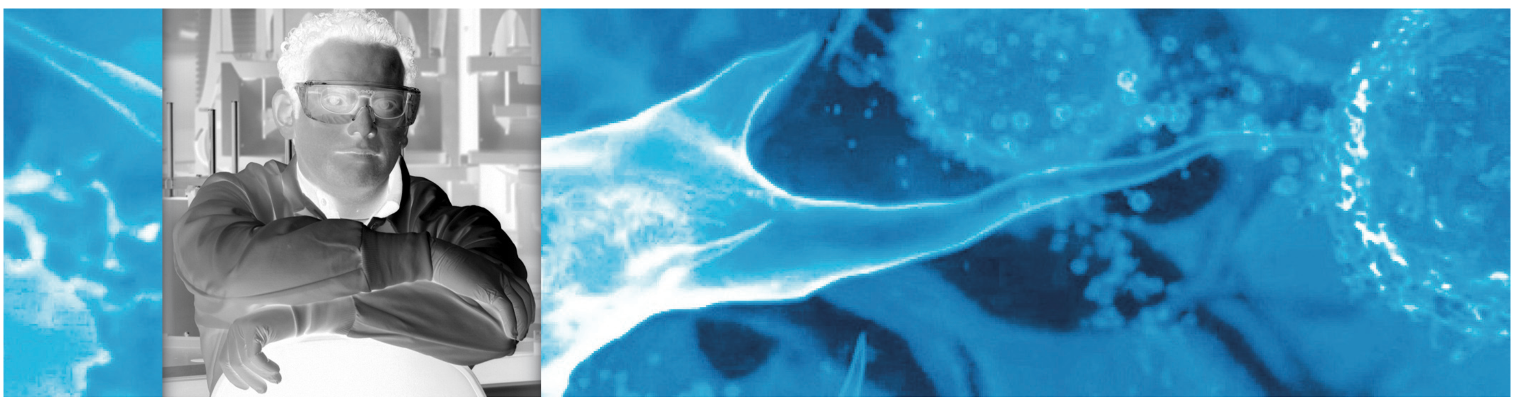
with a new looping algorithm, a new set of material parameters identified by research, and modifications to the mesh behavior.

With all this done, the image below indicates a perfect simulation in progress, with the ice detaching cleanly from the aluminum. No bending. No holes. No chipping. An almost perfect result.

As the simulation is perfected over time, it is no stretch to argue that we may shift from ice to more complex materials. Special thanks must be given to:

- Professor Raul Radovitzky
- Miss Zhiyi Wang (The graduate student behind most of the solutions and whose work I am reporting on)
- Miss Linsey Bjornstad (The graduate student who assisted in this project before me)

TRANSFORMING THE LANGUAGE OF LIFE INTO VITAL MEDICINES



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MURJ Reports

Real-Time Intervention Framework for Nicotine Poisoning via Identification of Alternate Compound and a Smart E-Cigarette Device

Divya Nori[1], Amanda Martinez[2]

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This research was not conducted in affiliation with MIT.

There has been a 200-fold increase in nicotine poisoning-related hospitalizations over the past decade which can be attributed to the rising popularity of electronic cigarette use or "vaping." E-cigarettes are battery-powered devices designed to vaporize a liquid that consists of lung-damaging additives, flavorings, and nicotine. Due to the potency and palatability of this vapor, users can easily ingest a dangerous level of nicotine and experience symptoms such as difficulty breathing, dizziness, and seizures. This paper proposes a smart e-cigarette device capable of tracking nicotine release with respect to time, stopping traditional vape liquid release when a threshold is reached, and switching to a safer compound. To find this alternate compound, two potential candidates – vanillin and menthol – were evaluated for their potential to cause lung damage and extent of thermal degradation. Through creation of a synthetic lung tissue-mimicking material and analysis of permeation, this study concludes that vanillin causes a significantly lower amount of lung damage in comparison to vape liquid. Additionally, it displayed low thermal degradation as evaluated through GC-MS analysis, establishing that vanillin is a viable alternate compound. Vanillin was therefore integrated into VapeSafe, a smart tandem e-cigarette device that detects dangerous nicotine use and intervenes in real-time by switching compound release.

1. Introduction

Over the past three years, the percentage of high school and college students who report vaping regularly has tripled, with 14% of U.S. college students reporting daily use of e-cigarettes (National Institute on Drug Abuse, 2019). Rates of e-cigarette use among high schoolers has risen from 1.5 percent to 16 percent between 2011 and 2015, and rates among middle schoolers have increased by 9 times (U.S. Food and Drug Administration, 2020). One major problem associated with the use of vape products is that nicotine is highly addictive, and users can easily become "nic-sick," which refers to symptoms experienced when nicotine beyond an individual's tolerance level is consumed (American Lung Association, 2019). America's top e-cigarette companies claim that one pod contains "as much nicotine as a whole pack of cigarettes," making it very easy to approach dangerous nicotine levels (American Lung Association, 2019). There were over 200 nicotine abuse-related hospitalizations per month in 2020, compared to only one nicotine-related hospitalization per month in 2010 (National Poison Data System, 2021). An approach by which nicotine abuse can be stopped in an automated fashion is essential to reduce the number of vape-related hospitalizations.

This study proposes a tandem smart e-cigarette device that contains regular e-cigarette liquid on one side and an alternative compound on the other. When a threshold volume of nicotine has been released within a given time span (individualized to the user based on tolerance), the device switches from releasing e-cigarette liquid to an alternative vapor, preventing nicotine poisoning in an automated fashion. This study seeks to identify a suitable non-addictive alternate compound that tackles the central problems presented by traditional vape liquid: degradation into toxic compounds and irreversible lung damage.

Traditional e-cigarettes contain over 7000 chemicals including diacetyl, formaldehyde, acrolein, and propylene glycol (National Academies of Sciences, 2018). Diacetyl is used to deepen e-cigarette flavors and has been shown to damage small passageways in the lungs. Formaldehyde has repeatedly been linked to lung/heart disease, and acrolein, a key component of weed killer, also damages the lungs. Prior literature attempts to identify alternatives to these compounds, but most proposed substances are VOCs that would still cause lung damage (Duell, 2019). In addition to parent compounds that cause physiological damage, most of these compounds degrade into other toxic substances when vaporized within the e-cigarette device (Duell, 2019). For example, citric acid has been proposed as an alternate compound and although it is inherently safe, it degrades into toxic citraconic anhydride after thermal exposure (Kaur, 2019). This study investigates the viability of vanillin and menthol as alternatives that display low thermal degradation and cause minimal lung damage. These compounds were selected for evaluation because they are similar in flavor to traditional e-cigarette liquids, so the user would not be able to detect a difference when the device switches compounds.

To evaluate the thermal degradation potential of the two experimental compounds, this study asks, what is the effect of thermal exposure on vanillin and menthol in terms of degradation? The experimental compounds' degradation was compared to a positive control (traditional vape liquid) and negative control (water), and the hypothesis was that both vanillin and menthol will display a significantly lower amount of degradation that the positive control. Additionally, to evaluate potential lung damage caused by the experimental compounds, this study specifically investigates: what is the effect of vanillin and menthol vapor on synthetic model lung tissue in terms of tissue permeation compared to traditional vape liquid? Both vanillin and menthol were hypothesized to display a significantly lower amount of model tissue permeation than traditional vape liquid.

2. Methods

Gas chromatography-mass spectrometry (GC/MS) is an analytical method used to identify different substances within a test sample. GC/MS was applied using CFM-ID to analyze the substances that the experimental compounds (vanillin and menthol) degrade into when heated. Five trials were run for each experimental compound and controls, the settings used are shown in Table 1. The number of peaks, relative intensity of peaks, and toxicity of components with highest intensity were analyzed.

Spectrum Type	Electrospray Ionization
Ion Mode	Positive
Adduct Type	[M+H]+

Table 1: Electrospray ionization spectrum type, positive ion mode, and [M+H]+ adduct type were applied for GC/MS analysis.

For the lung damage assessment, lung tissue was synthetically modelled by creating a lattice of air beads (alveoli) in aqueous solution. A density-driven approach was employed to develop a hydrogel-based lung tissue model. The standard density of the lung's posterior plane is 0.3 g/cm^3, and to mimic this density, a hydrogel with density 1.060 g/cm^3 was created and Styrofoam beads (0.003 g/cm^3) were suspended. The material's combined density was 0.28 g/cm^3. To prepare the gel, 714 ml of water and 80g of gelatin were heated to 50 degrees Celsius. Once the gelatin dissolved, 2g hydroquinone + 48 ml diH2O, 0.02g copper (II) sulfate pentahydrate + 30 mL diH_2O, and 0.353g of ascorbic acid + 50 mL diH_2O were added. Finally, 90g of methacrylic acid were added to the solution. The gel solution was poured over Styrofoam beads in small clear acrylic boxes, and the boxes rested overnight. To prepare each compound for evaluation, one drop of food coloring was added to 30 mL of dilute menthol, dilute vanillin, vape liquid, and water for visualization. All four solutions were vaporized and dispensed onto the hydrogel (4 trials for each). The lid of the acrylic box was then closed, and pictures were taken after twenty-minutes to assess which compound adhered most to the synthetic lung tissue. Image processing in Python (scikit-image) was applied for precise surface area analysis. Based on results from both the lung damage assessment and thermal degradation assessment, one experimental compound was integrated into the right side of the VapeSafe device.

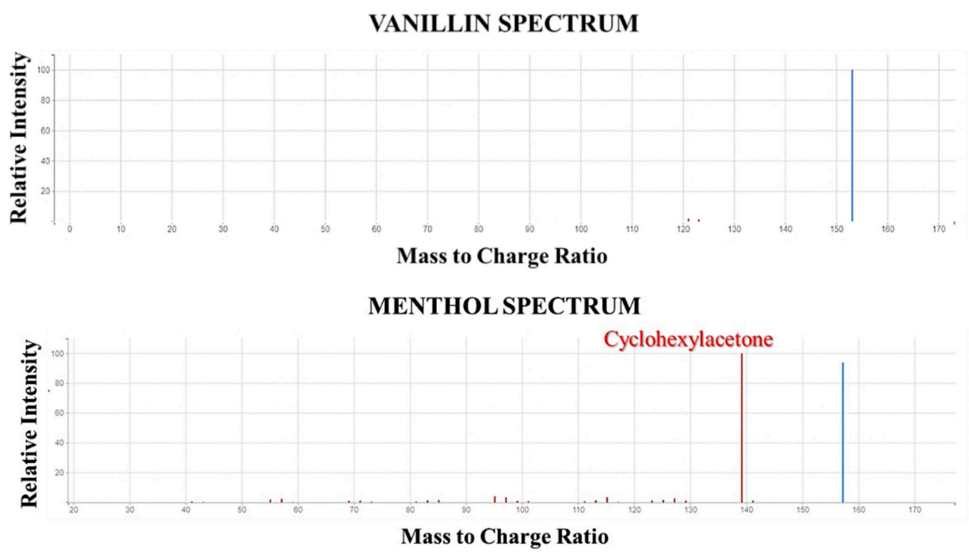
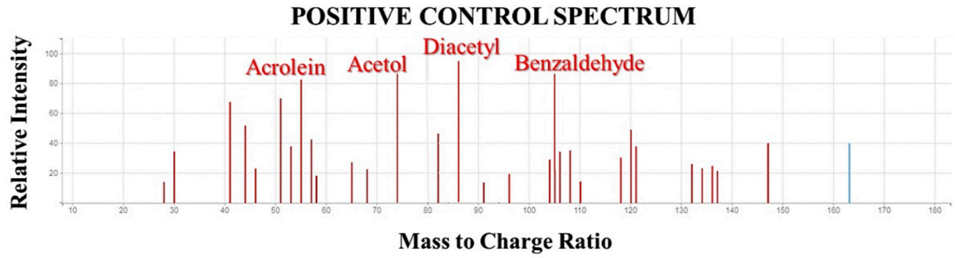


Figure 1 (top): Vanillin does not degrade into any new compounds with high relative intensity. The highest peak shown in blue represents the parent compound. **Figure 2** (bottom): Menthol degrades into one compound with high relative intensity, and this compound causes respiratory irritation.



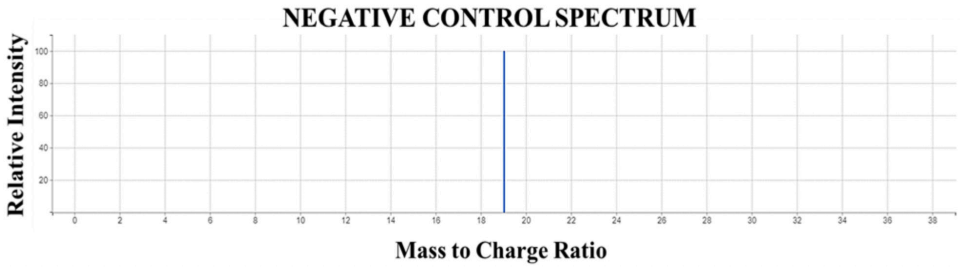


Figure 3 (top): Traditional vape liquid degraded into several compounds that have been linked to lung disease. The parent compound has a relative intensity of only 40%, meaning it degraded considerably. **Figure 4** (bottom): Water did not degrade into any new compounds as expected, making it an effective negative control.

3. Results

Figure 1 shows the GC/MS spectrum for vanillin, and the two small red peaks with a mass to charge ratio of approximately 120 indicate that vanillin degrades into two new compounds when heated. However, neither of the two new compounds have a high relative intensity. In comparison, Figure 2 shows that menthol degrades into 25 compounds when heated, but only one has high relative intensity. The compound with the highest relative intensity is $C_9H_{16}O$ (cyclohexylacetone) which causes respiratory tract irritation.

Figure 3 shows the GC/MS spectrum for traditional vape liquid (positive control), and this substance degraded into 31 new compounds with 4 of them having a relative intensity of greater than 80%. These compounds were C_3H_4O (acrolein), $C_3H_6O_2$ (acetol), $C_4H_6O_2$ (diacetyl), and C_7H_6O (benzaldehyde). The negative control's spectrum (water) displays no thermal degradation as shown in Figure 4.

Table 2 shows the means/SD of total peak counts and high intensity peak counts for the experimental compounds and controls. These values were used to run independent samples t-tests. As shown in Table 3, at a significance level of 0.01 and with 4 degrees of freedom, there is a significant difference in total number of peaks and high intensity peaks between vanillin and the positive control. There is a significant difference in high intensity peak count between menthol and the positive control but no significant difference for total peak count.

Sample	Sample Count (N)	Mean Peak Count (Rounded)	Standard Deviation of Peak Count	Mean High Intensity (>80%) Peak Count (Rounded)	Standard Deviation of High Intensity Peak Count
Vanillin	5	3	1.2	1	0
Menthol	5	26	1.8	2	0.3
Trad. Liquid	5	32	2.3	4	0.6
Water	5	1	0	1	0

Table 2: Across 5 trials for each compound, the mean peak count was greatest for traditional e-cigarette liquid and lowest for water. Menthol had a higher mean peak count (26) than vanillin (3). Similarly, for mean high intensity peak count, menthol had a higher mean (4) than menthol (2).

Sample	t-value for peak count	t-value for high intensity peak count
Vanillin w/ respect to positive control	**25.00**	**11.18**
Menthol w/ respect to positive control	4.59	**6.67**

Table 3: Bolded t-statistics values are significant at a significance level of 0.01 and with 4 degrees of freedom.

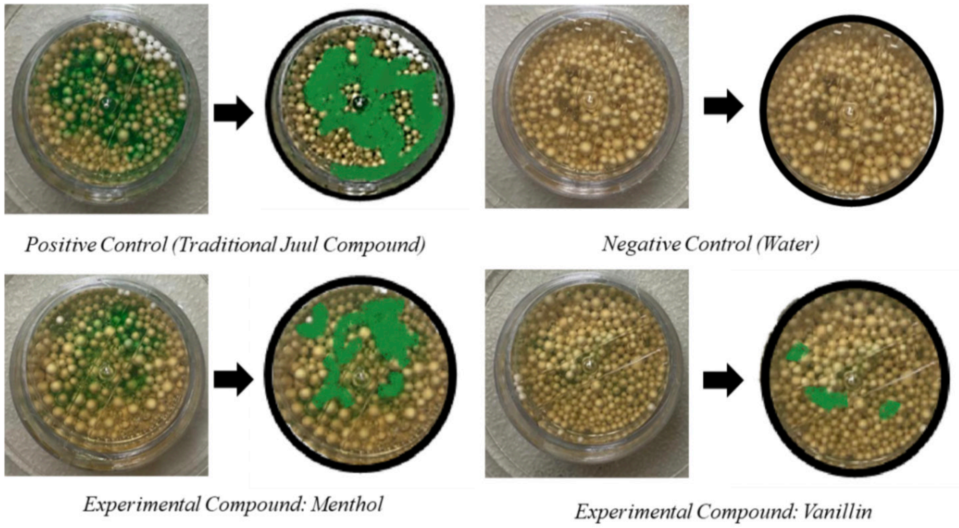


Figure 5: The surface area of synthetic lung tissue permeated by the compounds' vapor was highlighted computationally in Python. The positive control has the greatest highlighted area while the negative control has no highlighted area. The experimental compounds fall within these bounds.

Sample	Trad. Liquid	Menthol	Vanillin	Water
Affected Surface Area in Percentage Points (across 4 trials)	Mean: 73.9 SD: 5.6	Mean: 26.3 SD: 2.4	Mean: 7.4 SD: 1.3	Mean: 0.0 SD: 0.0

Sample	t-value
Menthol w/ respect to positive control	**15.6**
Vanillin w/ respect to positive control	**23.1**

Table 4 (left)**:** As computed in scikit-image, the traditional vape liquid had the highest affected surface area percentage. Menthol had the second-highest mean percentage (26.3%), and vanillin had a mean percentage of 7.4%. **Table 5** (right)**:** Bolded t-statistics values are significant at a significance level of 0.01 and with 3 degrees of freedom.

4. Discussion

In terms of thermal degradation potential, the t-test results provide preliminary confirmation that vanillin could be a safe alternative for traditional vape liquid. Given that there is a significant difference in high intensity peak count between menthol and the positive control but not for regular peak count, no definite conclusion can be drawn about the safety of menthol in terms of thermal degradation. Both compounds evaluated in this study display comparatively lower thermal degradation potential than previously investigated compounds. Previous studies rarely differentiate between high intensity peak count and total peak count. This added level of analysis provides some evidence of menthol's safety because there is a significant difference in high intensity peak count between menthol and traditional e-cigarette liquid.

Both vanillin and menthol display a significantly lower amount of lung tissue permeation than the positive control. When a t-test is run at a 0.1% significance level with 3 degrees of freedom to compare vanillin and menthol, the t-value exceeds the critical value. This indicates that vanillin displays a significantly lower amount of tissue permeation than menthol, so vanillin is the safest in terms of lung damage. The density-driven approach to model lung tissue has not been used to evaluate the effects of e-cigarette vapor before, though these results align with previous work showing that e-cigarettes cause lung damage.

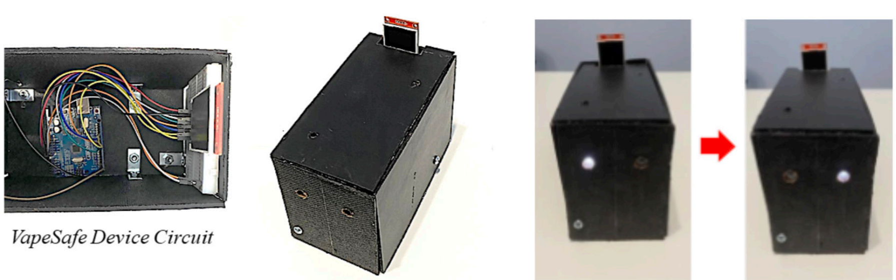


Figure 6: The VapeSafe prototype device hosts the traditional vape compound on the left and vanillin on the right.

5. Conclusions

This study provides preliminary confirmation that vanillin is a viable alternate compound for integration into a smart e-cigarette device in terms of both thermal degradation and potential for lung damage. Therefore, vanillin was integrated in the right compartment of VapeSafe, a smart e-cigarette proof-of-concept device that begins releasing the vaporized alternate compound when a threshold level of nicotine has been dispensed in a timespan to prevent nicotine poisoning. The prototype was built using an Arduino Uno and WiFi module as shown in Figure 6.

In the future, the lung damage assessment could be conducted on lung epithelial cells for more accurate results. A wider range of compounds could be tested as safer alternatives for traditional vape liquid including other diacetyl-free substances.

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