CURJ

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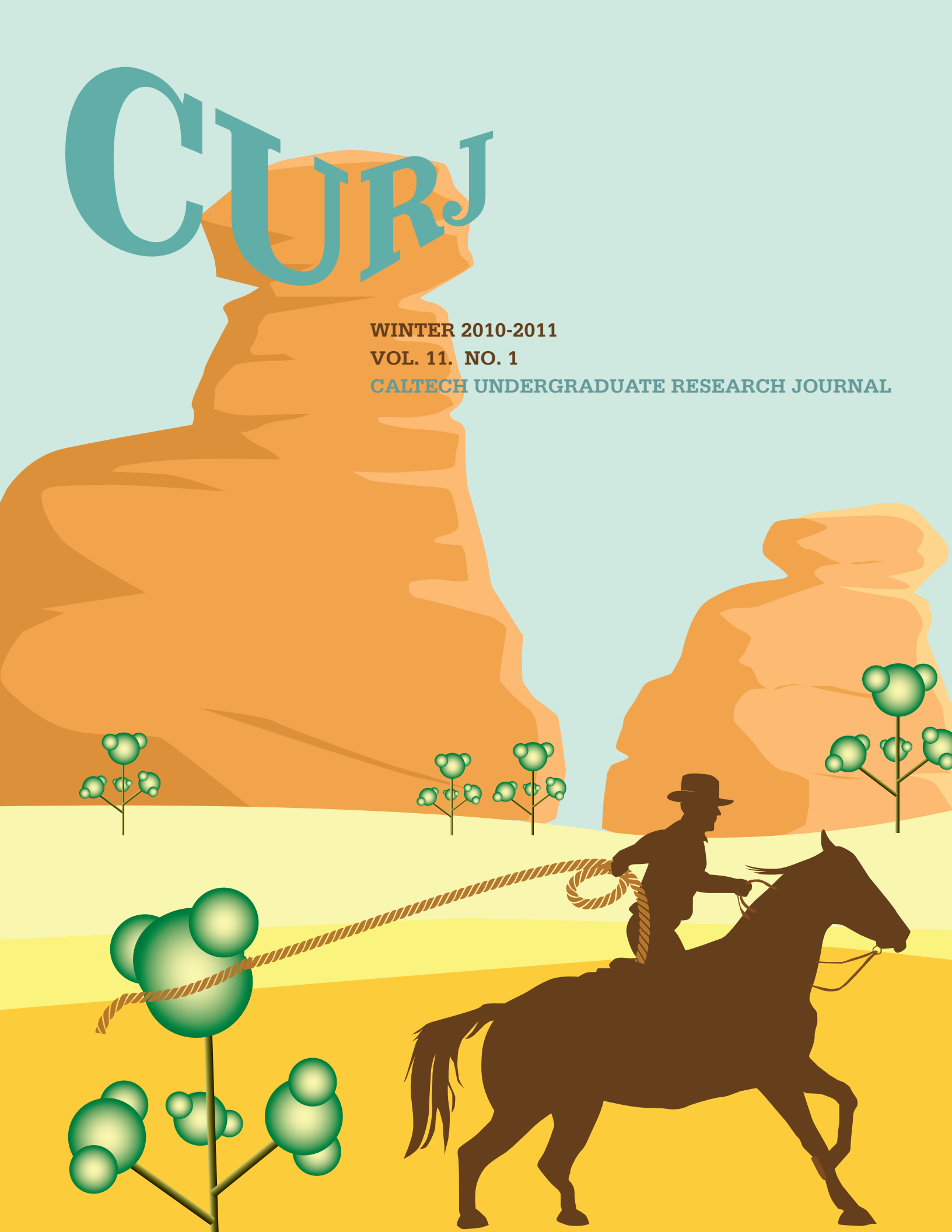

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CALTECH UNDERGRADUATE RESEARCH JOURNAL vol. 11. no. 1

From the editor

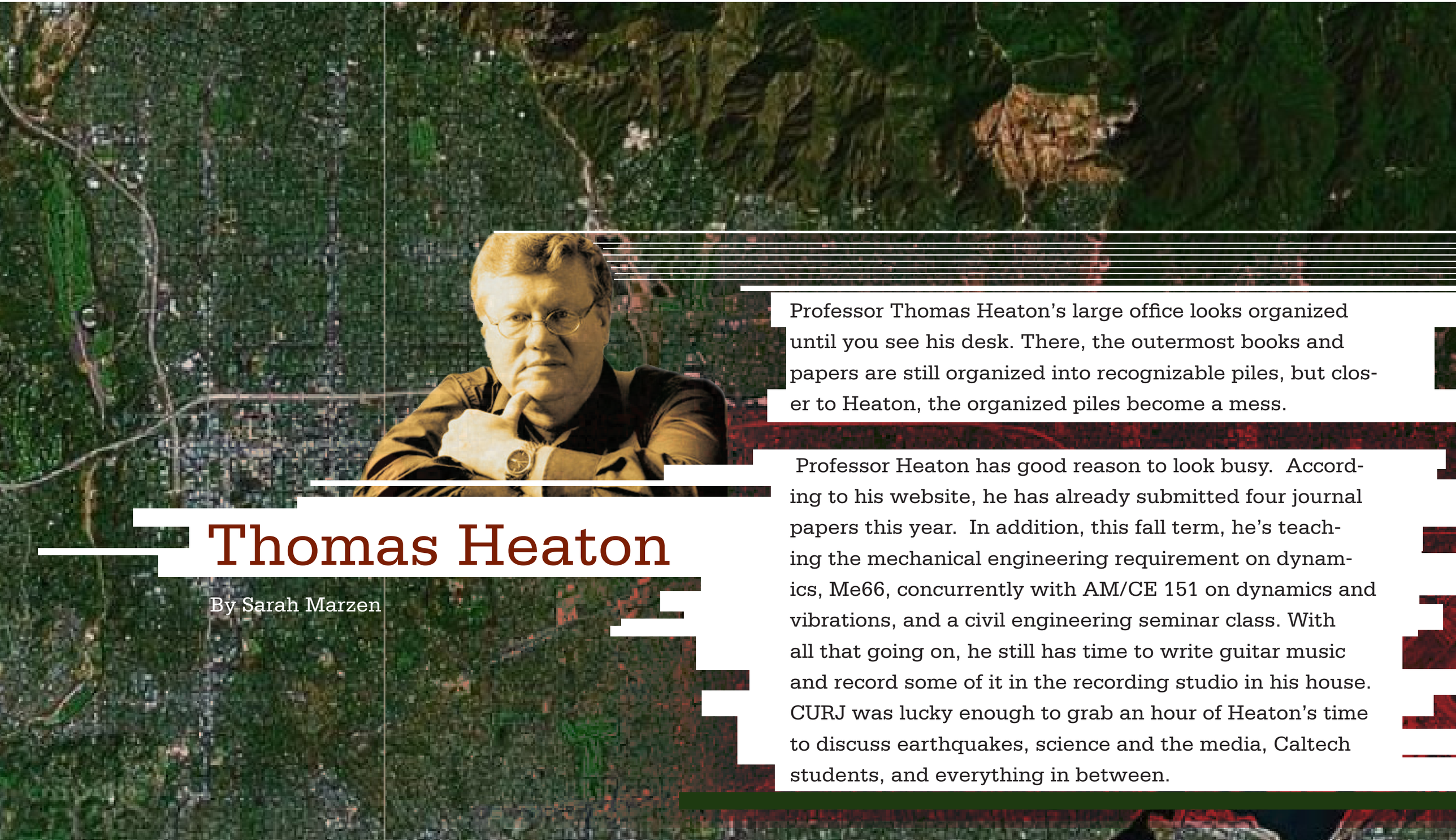
Welcome to the next issue of CURJ. As always, our journal highlights some of the best work being done by today's undergraduates, tomorrow's leading investigators. While CURJ will always be committed to supporting the next generation of scientists and innovators, it's something we can't do on our own. We need you—reading this journal right now—to be a part of our mission.

If you're a current undergrad, send us an email when your next project is written up; we'd love to showcase your work. If you're a research mentor, encourage your students to publish their work even in its earliest stages; we love to help nascent ideas develop. And if you're an aspiring scientist not yet in college, keep asking questions and exploring; we'd love to hear from you some day.
In the end, science does the most good when it's shared with the world, for others to understand and build on.

With those words in mind, I'd like to formally re-introduce the CURJ website (http://curj.caltech.edu), which has been completely redone for 2011. There, you can read past and present articles from CURJ, submit new articles for publication, apply to work with us, find resources for undergraduate research, and much more. Please take a look and let us know what you think.

Elizabeth Mak

Editor in Chief



Thomas Heaton

By Sarah Marzen

Professor Thomas Heaton's large office looks organized until you see his desk. There, the outermost books and papers are still organized into recognizable piles, but closer to Heaton, the organized piles become a mess.

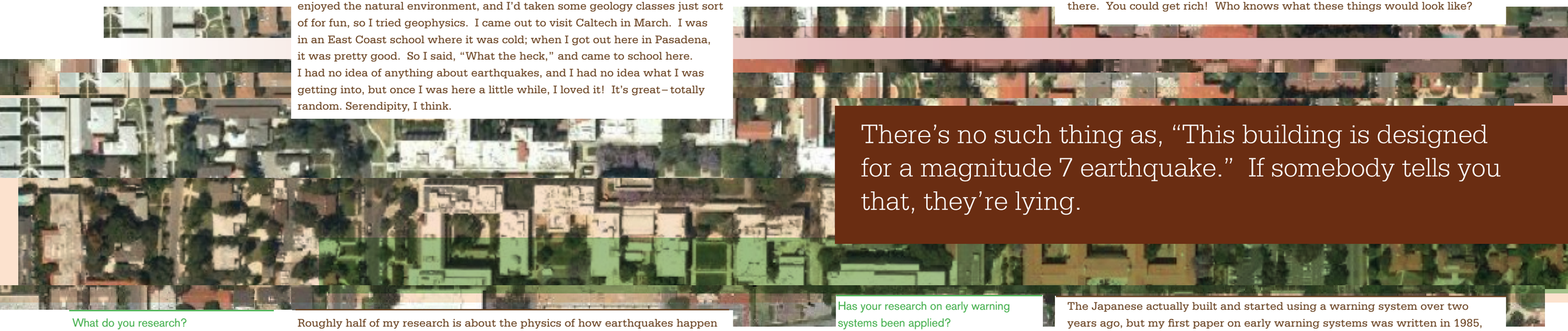
Professor Heaton has good reason to look busy. According to his website, he has already submitted four journal papers this year. In addition, this fall term, he's teaching the mechanical engineering requirement on dynamics, Me66, concurrently with AM/CE 151 on dynamics and vibrations, and a civil engineering seminar class. With all that going on, he still has time to write guitar music and record some of it in the recording studio in his house. CURJ was lucky enough to grab an hour of Heaton's time to discuss earthquakes, science and the media, Caltech students, and everything in between.

CURJ

How did you get into geology?

HEATON

Life is chaotic. I love music, but I'm not good enough to make a living out of it. And so I couldn't be a musician. I was a physics major as an undergraduate, but that was in the 1960's, and those days, the physics was all about high energy physics. But by 1972, when I graduated, they had more than enough people to do that. So when I applied to physics graduate schools. I got in, but those days they actually sent all of us letters that said, "You can come, but you'll never get a job. None of our graduates are getting any jobs in physics. We suggest you choose another field." So what do I do now? I'd always enjoyed the natural environment, and I'd taken some geology classes just sort of for fun, so I tried geophysics. I came out to visit Caltech in March. I was in an East Coast school where it was cold; when I got out here in Pasadena, it was pretty good. So I said, "What the heck," and came to school here. I had no idea of anything about earthquakes, and I had no idea what I was getting into, but once I was here a little while, I loved it! It's great – totally random. Serendipity, I think.



There's no such thing as, "This building is designed for a magnitude 7 earthquake." If somebody tells you that, they're lying.

What do you research?

Roughly half of my research is about the physics of how earthquakes happen and the other half i about the effects of earthquakes- how they affect buildings and how to make systems that react to earthquakes when they happen. We're working on early warning of earthquakes system that will tell you that the waves are on their way, seconds or minutes before the wave hits.

How do these early detection systems work?

Seismic waves generally travel at velocities of several thousand miles per hour, but radio waves travel even faster. If you have seismometers near where earthquake begins, you can send messages to some places and tell them the waves are on their way and will arrive shortly. Most of the time, when you feel an earthquake, it'll be a small earthquake nearby or a bigger earthquake from farther away. For those farther away earthquakes, we're working on early warning system that would say, "The waves are on their way to Pasadena. They'll get there in a minute. Make sure you're sitting some place quiet so you can enjoy the motion when it comes through." If it's a nearby earthquake, your cell phone might warn you, "Light shaking in 3, 2, 1." Then, after the shaking, it'd say, "Hope you enjoyed it!" Mostly people don't like earthquakes because even if it starts as light shaking, it could get nasty-- you don't know. But this early warning system would come on and tell you, "Don't have a cow! It's okay." In rare instances, it might come on and say, "You're toast. 3, 2,..." It seems like bad luck that the earthquakes we'd need most warning to prepare against are the same earthquakes that we'll only have a few seconds to prepare against. All kinds of systems now have computerized controls. Maybe we'll have early warning systems that will let you out on the nearest floor if you're in an elevator; or maybe they'll shut down the trains to avoid derailing the train tracks. Maybe these systems will trade all your stock so that you buy "Concrete Futures" or something before the waves actually get there. You could get rich! Who knows what these things would look like?

Has your research on early warning systems been applied?

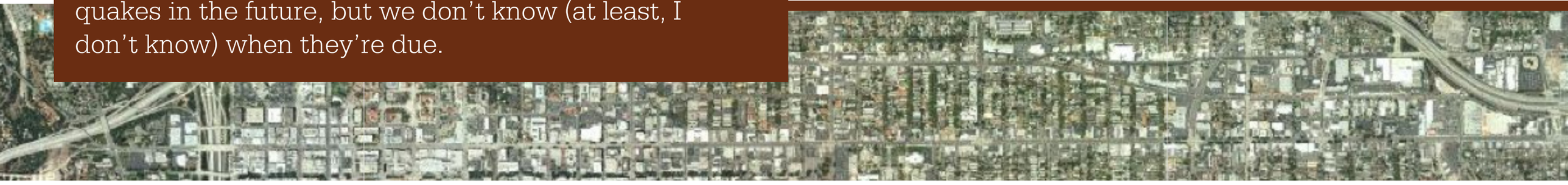
The Japanese actually built and started using a warning system over two years ago, but my first paper on early warning systems was written in 1985, so it's been a while coming. Now we're building an early warning system for California. My research is also used in the design of tall buildings, but probably my research is used less than I'd like. The people who build tall buildings don't necessarily want to hear what I have to say. Lots of buildings were constructed with inadequate welding procedures and those buildings are just sitting there, waiting for the welds to fracture. When they do, it makes them far more susceptible to collapse in a large earthquake.

How will Caltech's buildings do in an earthquake?

Caltech has a lot of older buildings made out of concrete, but our buildings are almost entirely sheer-walled buildings, which actually do extremely well in earthquakes. The new Cahill building is a concrete frame building, but the many columns in that are enormous with very carefully placed steel. Cahill's the only concrete-frame building on campus. The earthquake engineering department here at Caltech tended to steer the architecture away from those types of buildings. The design of the buildings is actually done by an outside professional engineering company, but they're told to go to 50% more than the code for earthquake safety, and then they're told that their plans will be reviewed by the engineering department at Caltech. So they tend to come up with pretty conservative designs for the structures. In the end, I guess somebody decided that it was more important to have an understandable architectural style for the Cahill building.

"It's overdue." I have no idea if it—the earthquake—is overdue or not. We know there will be more earthquakes in the future, but we don't know (at least, I don't know) when they're due.

There are no buildings on rollers.



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Is there a big earthquake coming soon to Southern California?

HEATON

Of course, now is closer to the earthquake than it was yesterday. But we have no idea. When I first came here in 1972, one of the field technicians said to me, "Tom, I've seen three generations of seismologists go to their graves with their dying words being 'It's going to go, it's going to go!'" That was 37 years ago and here I am. At this point in my career I'll tell you it's going to go, but you could get pretty old waiting for a really big earthquake. You can't wait around for them. You just have to keep at it in terms of planning for the next one, and it'll take you by surprise when it does come.

CURJ

Have we improved in our building design since the devastating San Francisco earthquake in 1906? Should we feel a little bit safer?

HEATON

Many things have improved but probably some things have gotten worse. There were never any really tall buildings or large bridges in 1906, and those tall buildings and large bridges react to the low frequency part of the ground shaking. A really large earthquake is rich in low-frequency ground motion. We've never had a city with tall structures go through a really large earthquake, and the simulations that we do here at Caltech suggest that there may be some pretty serious problems. Generally our shorter structures are better than they used to be. We don't have too many unreinforced brick buildings, and those are our most vulnerable buildings. The buildings that are most likely to kill people are the buildings that are six to twenty story concrete buildings with concrete columns instead of concrete walls.

CURJ

Here's something that's always confused me. What do those Richter scale magnitudes mean? They don't seem to be directly related to the damage done by the earthquake.

HEATON

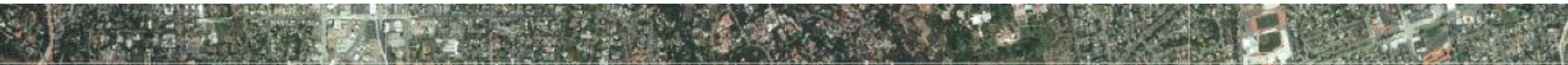
Originally, when people talked about the size of the earthquake, it was based on how much damage was done by the earthquake. But Richter said, that doesn't tell us much from a scientific point of view. Damage depends on how strong the buildings are, whether the buildings are close to the earthquake, and what kinds of buildings are there. The Richter scale was originally designed to separate the damage part of the measurement from the basic measurement of the earthquake itself. Scientists have worked hard to understand what those measurements of the Richter scale mean. You could think of it as the logarithm of a total energy in an earthquake, but I'd have to spend a couple hours explaining how we define energy. Unfortunately, we spend half our time trying to explain to the general public what a logarithm is.

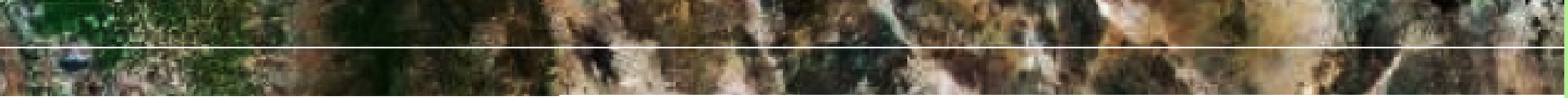
CURJ

Is there a general misconception about earthquakes that you'd like to dispel?

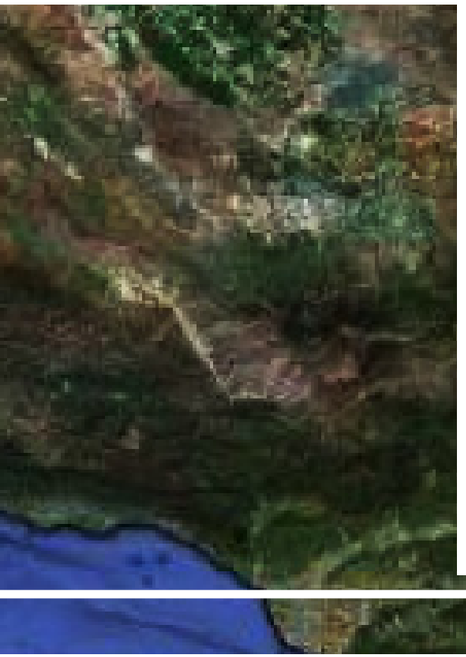
HEATON

Earthquakes are a very mysterious scientific phenomenon. At this point in time, we know there is very low friction deep in the Earth while the plates are sliding, but we don't know how. The implications of the sudden changes in frictional properties have profound implications for how earthquakes work and just how the Earth deforms in general. Trying to simulate this in a laboratory is almost impossible. At the depth of an earthquake, the pressure holding the rocks together is three times the pressure in the deepest part of the Marianas Trench. If you try to slide things past each other at those pressures in the laboratory, you almost instantly melt the rock due to frictional heating of the rock. But when we look at real faults, we don't find any melted rock. The implication is that somehow, the friction somehow instantly transitions to low friction during an earthquake, like you're ice skating. There are about half dozen speculated-on mechanisms, but none of them are a sure thing-- we don't know the mechanism.





What makes earthquakes so difficult to understand?



In the earthquake business, when I started out, people just said, "Well, the plate tectonics strains up the rocks, the energy's stored up, and then it breaks into an earthquake." But the more we've studied the process, the more we realize that's a really naive picture of how things actually fracture. It really gets into the question of how do things fracture and fail. You can't put the entire Earth into a machine and say, "When you push on it at this strength, then it's going to get a failure of this size when the stress reaches this point." You've somehow got to build up from looking at the microscale that you can touch with your fingers as a human being and figure out what the macroscale's going to look like. In many kinds of materials science problems it's just the opposite-- you take a piece of steel or glass, go into the laboratory, and pull on it until something happens, and then try to figure out what's happening at the molecular scale. To go from what's happening at the molecular scale up to the scale of the test equipment is a very challenging problem in science at the moment. In earthquake science, we've got the same kind of problem, except that we can test at the scale of the laboratory and we're trying to infer what the Earth looks. We're finding that the natural world is controlled by highly nonlinear chaotic systems, which are the forefront of the challenge of basic science. For any of the students interested in physics and mechanics: many things appear fractal, but to derive from first principles where that fractal geometry came from is usually an extremely challenging problem. It's the kind of problem that you'll win a big prize for solving. That kind of problem is very fundamental to the earthquake problem.

One of my favorites is that after every earthquake, someone will come up to me and say, "Isn't it a coincidence? You know, I saw you just the day before that earthquake." And every time somebody tells me that, I don't even know what to say. Now I reply back to them, "Yeah, isn't that amazing?"

CURJ

HEATON

How do you like teaching?

I like teaching quite a bit. But as long as I'm talking to the undergrads, I have to tell you, Caltech is not a correspondence school. These days I don't often like to teach undergraduates because often, they don't come to class! So if I have my two cents about teaching, it's that if I'm going to show up to class, the undergraduates should show up to class too. Another style of teaching is to have well organized notes and a really well organized website on the class so somebody can get everything they need to out of class without even showing up to class. That's not my classes. Just look at my desk! I'm just not that organized. If someone wants to take the class from me in that way, it's probably going to be frustrating.

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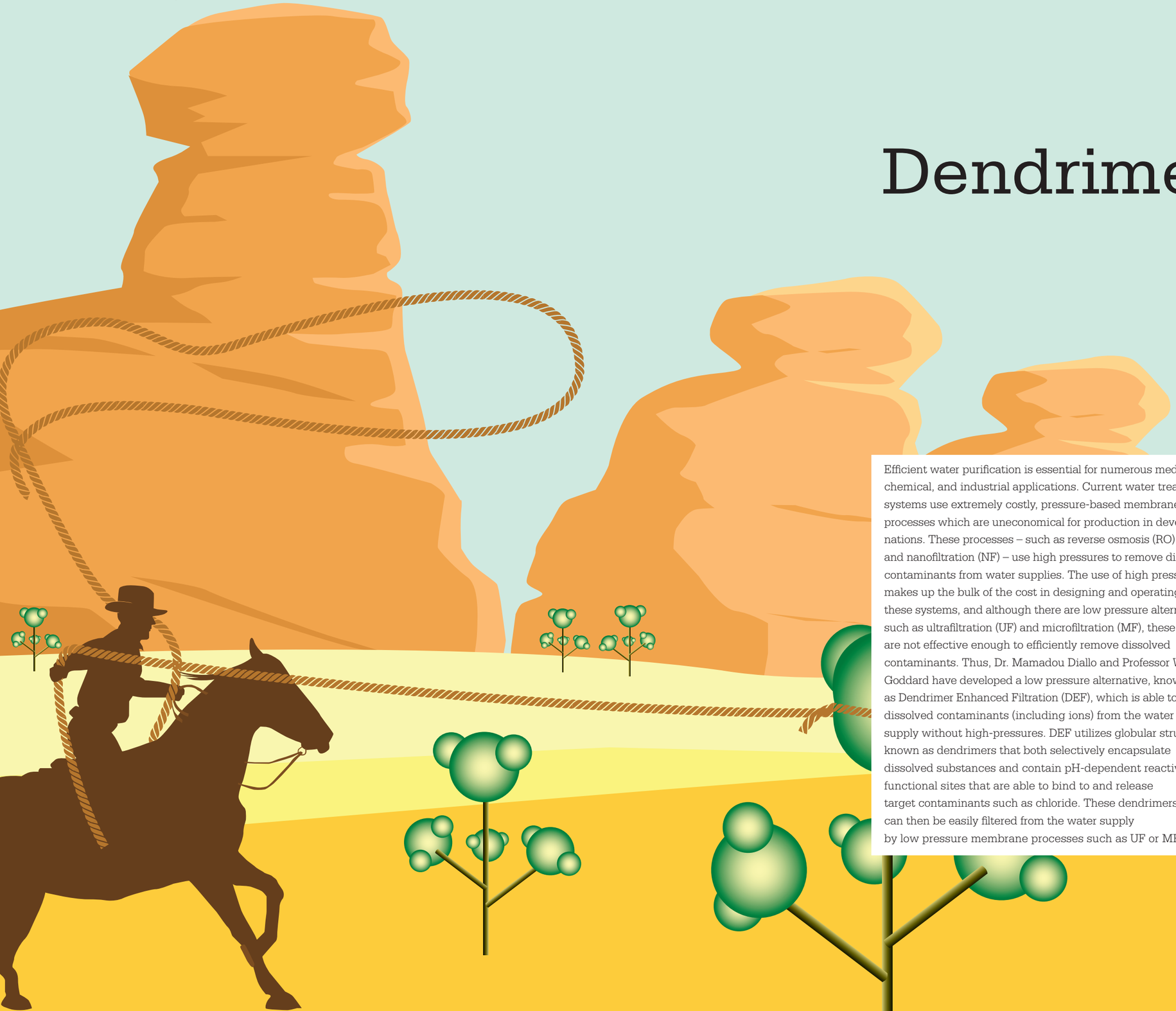
Dendrimer-Enhanced Filteration

A Novel Idea For Chloride Removal

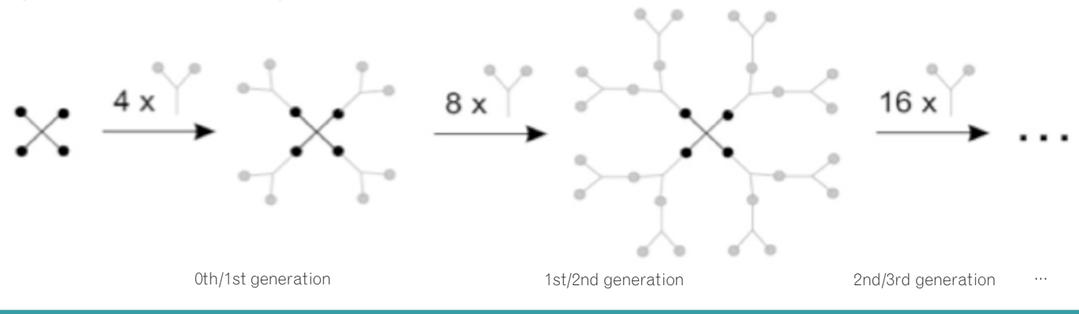
Author: Neha Samdaria
Mentor: Professor William A. Goddard III
Co-Mentor: Dr. Mamadou Diallo



Efficient water purification is essential for numerous medical, chemical, and industrial applications. Current water treatment systems use extremely costly, pressure-based membrane processes which are uneconomical for production in developing nations. These processes – such as reverse osmosis (RO) and nanofiltration (NF) – use high pressures to remove dissolved contaminants from water supplies. The use of high pressure makes up the bulk of the cost in designing and operating one of these systems, and although there are low pressure alternatives such as ultrafiltration (UF) and microfiltration (MF), these systems are not effective enough to efficiently remove dissolved contaminants. Thus, Dr. Mamadou Diallo and Professor William Goddard have developed a low pressure alternative, known as Dendrimer Enhanced Filtration (DEF), which is able to remove dissolved contaminants (including ions) from the water supply without high-pressures. DEF utilizes globular structures known as dendrimers that both selectively encapsulate dissolved substances and contain pH-dependent reactive functional sites that are able to bind to and release target contaminants such as chloride. These dendrimers can then be easily filtered from the water supply by low pressure membrane processes such as UF or MF.

In this study, we focused on the quantitative analysis of the effectiveness of dendrimer–anion interactions and their subsequent removal from the water supply. In particular, we were interested in investigating the removal of chloride anions for the desalination of water. We used a combination of acid-base titrations, ultrafiltration experiments, and ion chromatography to measure the binding of chloride to a G5-NH_2 Polypropyleneimine (G5-NH_2 PPI) dendrimer and a G4-NH_2 Polyamidoamine (G4-NH_2 PAMAM) dendrimer in aqueous solutions. From these measurements, we extracted the Extent of Binding (EOB) and Fractional Binding (FB) of the dendrimers and analyzed these values using an Extent of Protonation model. We discovered the G4-NH_2 PAMAM dendrimer bound more chloride ions than the G5-NH_2 PPI dendrimer, making it more effective in chloride removal processes. We can now expand current molecular dynamic simulation models to incorporate similar binding mechanisms and to improve water purification dendrimers.

Figure 1: The formation of dendrimer generations



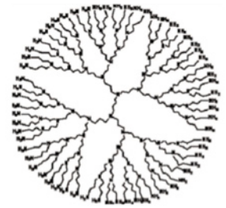
The mechanism of selective chloride encapsulation and removal

Dendrimer synthesis begins with a core molecule which is reacted with other monomers to yield a "zeroth generation" or "first generation" dendrimer (the terminology for naming dendrimers evolved over time). In this way, the dendrimer grows outwards, and each generation forms on a new layer of monomers – **Figure 1.**

In our experiment, we apply UF to a fifth generation polypropyleneimine (G5-NH_2 PPI) dendrimer – **Figure 2a** – and a fourth generation polyamidoamine (G4-NH_2 PAMAM) dendrimer – **Figure 2b** – to test the removal of chloride ions from water. There are two primary properties of these dendrimers that make them efficient in purifying chloride-contaminated water:

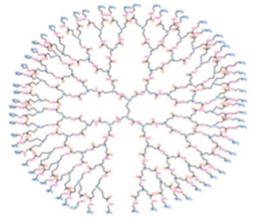
Figure 2: Water-soluble dendrimers

a.



a. G5-NH_2 PPI dendrimeer - 64 terminal NH groups, 62 internal NH groups, and 62 internal tertiary amine groups [A1,1]

b.



b. G4-NH_2 PAMAM dendrimer - 64 terminal amide groups, 124 internal amide groups, and 62 internal teriary amine groups [A1,1]

1. Both dendrimers undergo pH-dependent protonation which is the central mechanism for the capture and release of chloride ions. The amine groups on the dendrimers are able to ion-pair with chloride at a low pH (when the NH_2 groups are protonated) and release chloride at a high pH (when the NH_2 groups are neutral and can no longer exert the same electrostatic forces of attraction). As we increased the pH of the anion-dendrimer solution, we discovered a gradual decrease in chloride binding. This trend could be directly correlated with the Extent of Protonation (EOP) of each dendrimer as a function of pH. Using the Henderson-Hasselbach equation, the EOP of a dendrimer can determine the fraction of functional sites that are available to participate in ion-pairing at any given pH, directly relating to how efficiently the compound is able to bind and remove chlorine ions from water. By multiplying calculated EOP values with the total number of NH_2 groups present on each dendrimer, we were able to determine the 'total number of protonated amines' as a function of pH for both dendrimers, which is useful for EOB and FB calculations.

2. A second type of binding occurs specifically between the chloride and the amide groups present on the G4-NH_2 PAMAM dendrimer. This binding interaction is pH-independent because it involves hydrogen bonding rather than ion-pairing. We postulated that each chloride would bind to one amide group, thus making 124 additional functional sites on the G4-NH_2 PAMAM dendrimer. Our experimental results supported this hypothesis since the G4-NH_2 PAMAM dendrimer bound 5x more chloride than the G5-NH_2 PPI dendrimer.

These two chemical properties of the dendrimers, combined with their physically large size, allowed us to filter them out of aqueous solutions using UF membranes with 1000 Dalton pores, eliminating the need for high pressure membrane processes. We performed our experiments using acid-base titration and UF and carried out chloride concentration analysis using Ion Chromatography (IC). Dendrimer-chloride solutions were generated using a fixed concentration of the dendrimer and chloride and varying amounts of Sodium Chloride (NaCl), Hydrochloric Acid (HCl) and Sodium Hydroxide (NaOH) in order to create solutions with different pHs. The chloride concentration of these solutions was then analyzed using IC, both before and after UF. The difference in the two concentrations yielded the amount of chloride that was bound to the dendrimer. From this, the EOB – **Figure 3a** – and FB – **Figure 3b** – were calculated using the following two equations:

$$FB = \frac{(C_{initial\ chloride} - C_{final\ chloride}) * 100}{C_{initial\ chloride}}$$

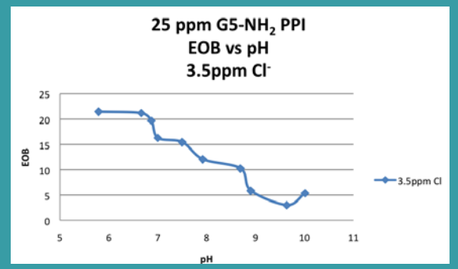
$$EOB = \frac{C_{initial\ anion} - C_{final\ anion}}{C_{dendrimer}}$$

Where: $C_{initial\ chloride}$ = initial chloride concentration (moles/L)
$C_{final\ chloride}$ = final chloride concentration (moles/L)
$C_{dendrimer}$ = Dendrimer concentration (moles/L)

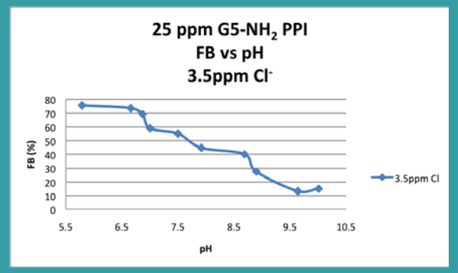
These two values were indicative of the binding ability of the dendrimer (reflected in the EOB), and its efficiency in encapsulating chloride ions (reflected in the FB).

Figure 3 – G5-NH_2 PPI binding to 3.5ppm Chloride

a.



b.

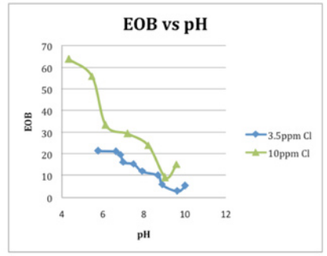


a. EOB vs pH - 25ppm G5-NH_2 PPI binding to 3.5ppm Chloride. We see a level EOB until pH 6.6 where it decreases suddenly due to the deprotonation of the internal tertiary amines, then a gradual decline until pH 8.69 where the EOB drops steeply due to the deprotonation of terminal NH groups.

b. FB vs. pH - 25ppm G5-NH_2 PPI binding to 3.5ppm Chloride. We see a level FB until pH 6.6 where it decreases suddenly due to the deprotonation of the internal tertiary amines, then again a gradual decline until pH 8.69 where FB drops steeply due to deprotonation of terminal NH groups.

Figure 4 – Increasing the APL to 10ppm Chloride (Cl-)

a.



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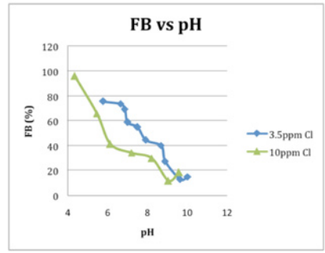


a. EOB vs pH - 25ppm G5-NH_2 PPI binding to:
* 3.5ppm Cl- (avg. APL ≈ 27)
* 10ppm Cl- (avg. APL ≈ 80)

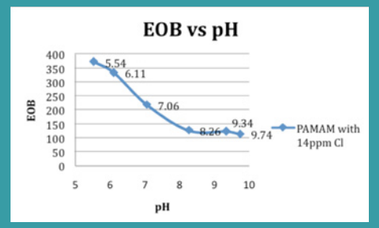
b. FB vs pH - 25ppm G5-NH_2 PPI binding to:
* 3.5ppm Cl- (avg. APL ≈ 27)
* 10ppm Cl- (avg. APL ≈ 80)

In low pH solutions, the FB was high enough to show the dendrimer's binding mechanism was quite efficient.

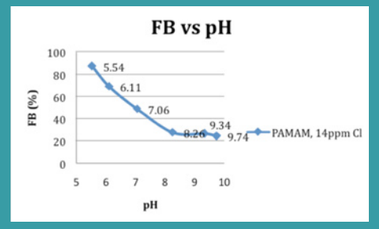
Decreasing EOB and FB are correlated to a rising pH for both dendrimers because the total number of amine groups that are protonated decreases as the pH increases. By observing Figure 3a, were also able to conclude that since only 21 chloride ions were being bound per dendrimer (at low pH) the dendrimer was unsaturated (assuming that each amine binds one chloride ion). We proceeded to increase the Anion-Polymer-Loading (APL), i.e the moles of anion/moles of dendrimer, to attempt saturation of the dendrimer. We progressively increased the APL from 27 to 80 – **Figure 4.**

Figure 5 – G4-NH_2 PAMAM binding to 14ppm Chloride

a.



b.



a. EOB vs pH – 12.5ppm G4-NH_2 PAMAM binding to 14ppm Cl- (avg. APL ≈ 451). Although the trend between this graph and Figure 3a are the same, these values are all significantly increased indicating a much higher EOB overall for the G4-NH_2 PAMAM dendrimer.

b. FB vs pH – 12.5ppm G4-NH_2 PAMAM binding to 14ppm Cl- (avg. APL ≈ 451). These values are very similar to the values obtained in Figure 3b,indicating a very similar FB for both dendrimers, and, therefore, a very similar extraction efficiency.

We were able to obtain 63% saturation by loading 10ppm Chloride onto 25ppm of the G5-NH_2 PPI dendrimer – **Figure 4**. At this low pH and with this level of saturation, the FB was calculated to be 95%, indicating that almost all the chloride present was being encapsulated by the dendrimer. Thus, the entire system is extremely efficient, which is a key variable in designing viable water purification systems. We repeated the experiment with the 12.5ppm G4-NH_2 PAMAM dendrimer loaded with 14ppm Chloride to investigate the effect of internal amide groups on dendrimer-chloride binding and efficiency. This high loading level yielded pHs low enough to observe chloride binding and exploited the hydrophilic nature of the G4-NH_2 PAMAM dendrimer, making it more suitable to higher chloride concentrations. We observed a significant increase in both the EOB – **Figure 5a** – and the FB – **Figure 5b** – compared to the G5-NH_2 PPI dendrimer due to the presence of the many amide groups.

We concluded that the 124 amide groups present in the G4-NH_2 PAMAM dendrimer[A1] were responsible for the high EOB values, even in high pH solutions. At a high pH, the terminal NH_2 groups and the internal tertiary amines are deprotonated. Since both dendrimers contain the same number of terminal NH_2 groups and internal tertiary amines[A1], the resulting difference in binding can be accounted for, in part, by the binding of tertiary amines to chloride in the G4-NH_2 PAMAM dendrimer.

But water molecules are free to bind chloride…

It is interesting to observe from Figure 5a that at low pH (≈5), the G4-NH_2 PAMAM dendrimer encapsulated approximately 370 chloride ions, whereas it only contains a total of 250 functional sites available to bind chloride ions (64 terminal NH_2 groups + 62 internal tertiary NH_2 groups + 124 internal amide groups). Thus, there were approximately 120 chloride ions being bound per dendrimer at low pH that could not be accounted for by any of the functional sites present in the dendrimer. Part of the explanation as to why there was extra chloride binding is that at a low pH (≈5), the G4-NH_2 PAMAM dendrimer traps approximately 325 water molecules. Encapsulated water molecules have a lower free energy and participate in hydrogen bonding with chloride ions readily. One chloride ion is coordinated with approximately 5 water molecules[4]; thus, this water coordination can account for approximately 60 additional chloride ions being bound to the G4-NH_2 PAMAM dendrimer at a low pH. This mechanism of water encapsulation is not present in the G5-NH_2 PPI dendrimer for two reasons: Firstly, this dendrimer is much smaller than the G4-NH_2PAMAM dendrimer[A1]; and secondly, this dendrimer is more hydrophobic due to the presence of propyl chains which link the tertiary and primary amine groups together. However, even after taking water encapsulation into consideration, we found that there were still approximately 60 chloride ions unaccounted for bound to the G4-NH_2 PAMAM dendrimer. Thus, we concluded that there were aspects of the binding mechanisms between the chloride and dendrimer, and, more importantly, between chloride and encapsulated water molecules that could not be precisely explained with current models. Further research will need to be carried out in order to investigate these mechanisms.

More than just a drop in a bucket.

Our results can be used to both enhance our understanding of the binding mechanisms utilized by various dendrimers in water purification processes and to expand current molecular dynamic simulation models. Preliminary results showed that these models assumed the binding capacity of some dendrimers, such as the G4-NH_2 PAMAM dendrimer, to be fulfilled when enough chloride was added to achieve dendrimer electro-neutrality. However, we show that these binding estimates may not be accurate, and that current models need to be modified in order to provide a more accurate simulation of the binding abilities of certain dendrimers. In order to effectively remove anions from water supplies such as groundwater and seawater using DEF, a thorough understanding of the binding mechanisms of dendrimers is required. Our results analyze the properties of dendrimers that make them so effective in chloride removal. In the future, these results will be incorporated into less expensive dendritic polymers and provide a step toward finding a solution to the global water purification crisis that exists today.

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Acknowledgements

We acknowledge Dr. Mamadou Diallo, Dr. CJ Yu, and Dennis Chen for their suggestions about experimental procedures and initial analysis. We also acknowledge Dr. Nathan Dalleska for his guidance in using the Ion Chromatography machine.

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Outlining the Superhighways of the Brain

Written by: Joe Funke

Introduction

The brain is easily the most complicated organ of the human body, and scientists are still trying to understand its complex signal processes and functions. It controls everything from walking up the stairs to driving a car, and without a centralized nervous system, our lives would not be as we know it.

Understanding the brain involves understanding the pathways or connecting fibers between different regions of the brain. Some of the regions include the cerebellum, cerebrum, medulla, and hypothalamus, which are all important for day-to-day function. When different regions of the brain communicate abnormally, psychiatric illnesses may develop. Therefore, it is important for us to understand how different areas of the brain interact.

"When different regions of the brain communicate abnormally, psychiatric illnesses may develop."

"In theory, this should make the probabilistic algorithm more precise than the deterministic algorithm."

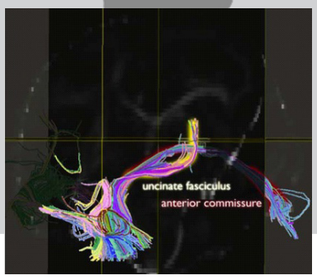

Figure 1. Location of the uncinate fasciculus in the macaque brain found through diffusion magnetic resonance and the message passing-based algorithm. The uncinate fasciculus is highlighted in gold and the anterior commissure is highlighted in red as a reference.

A Different Way of Thinking

Currently, scientists use high-resolution diffusion-weighted magnetic resonance images to see the connecting fibers in the brain. Through high-powered magnetic fields, electrons of the water molecules in the brain align with the fibers in the brain, allowing the magnetic resonance imaging (MRI) machine to capture the regions where the water molecules are aligned. High-resolution diffusion-weighted MRI involves a deterministic fiber tracking algorithm that measures the diffusion patterns of the water molecules through such diffusion MRI scans. This algorithm separates the brain into discrete quantities called voxels, which are three-dimensional equivalents to pixels on a computer screen. This method determines the primary diffusion direction in each voxel, and then tracks these directions through neighboring voxels to build a hypothetical fiber tract.

We propose a new algorithm that is much more accurate and precise. We introduce the probabilistic message passing-based algorithm that accounts for multiple diffusion directions, and thus multiple fiber tracts in each voxel. This algorithm then probabilistically determines the direction of diffusion after considering all the voxels in the region. In this method, more information is preserved as compared to the deterministic approach; not only is the primary diffusion pattern recognized, but other possible diffusion directions are considered as well. In theory, this should make the probabilistic algorithm more precise than the deterministic algorithm.

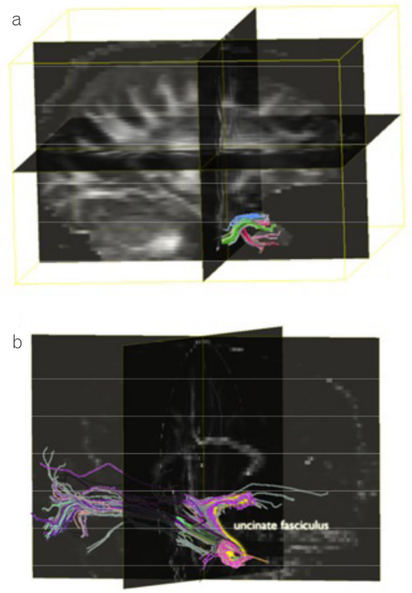

Figure 2. Uncinate fasciculus shown in the low-resolution human brain through diffusion magnetic resonance. (a) The deterministic approach did not locate the uncinate fasciculus. (b) The message passing algorithm did locate the uncinate fasciculus highlighted in gold. A threshold was used to reduce the number of fibers shown.

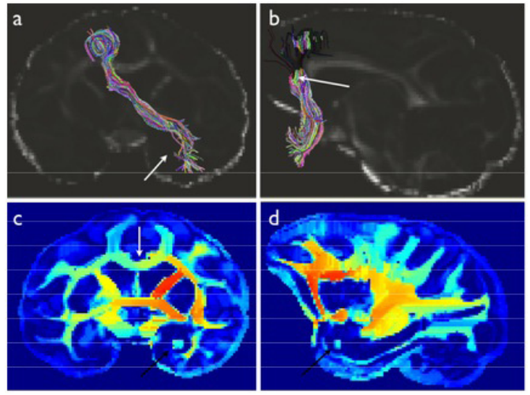

Figure 3. Possible amygdala-sgACC connection in the high-resolution macaque brain. (a) A coronal view shows the visualization of the connective fibers indicated by the white arrow. (b) A sagittal view shows the visualization of the connective fibers indicated by the white arrow. (c) A coronal view of the raw data probability distribution. Warm and cool colors represent the higher and lower likelihood of the correct connective tract. The amygdala is indicated by the black arrow. (d) A sagittal view of the raw data probability distribution. The amygdala is indicated by the black arrow.

Results using the message passing algorithm on the macaque brain are displayed in Figure 3. A sagittal view, dividing the brain into left and right (Figure 3c), and coronal view, dividing the brain into front and back (Figure 3d) are taken of the macaque brain and displayed as probability maps. The regions with warmer colors indicate the higher likelihood of the presence of amygdala-connecting fibers and cooler colors represent lower probability areas. By tracing the highest probability areas, we can create a flow field visualizing the hypothesized fibers. These fibers are shown in Figures 3a and 3b. Interestingly, we notice that the uncinate fasiculus does not extend completely to the superior sgACC in the human brain. This suggests that the uncinate fasiculus connects to another fiber tract that leads to the sgACC. However, we do see that the uncinate fasiculus leads directly to the sgACC in the macaque brain.

To validate the accuracy of this approach compared to the deterministic algorithm, we looked at different regions of the human brain simultaneously. By visual inspection, we see that the probabilistic approach shows many thin, densely-packed fibers in almost all of the regions (Figure 4a). In comparison, the deterministic approach shows thick and sparse fibers in the same regions (Figure 4b). To quantify the results of the connective fibers, we averaged the length of each fiber for the different regions for each of the algorithm results. In comparison, the probabilistic algorithm found more fibers in seven of the eight tested regions, and those fibers were longer in five of the eight regions on average (Figure 5).

Putting it to the Test

This new algorithm is meant to better detect possible fiber tracts within the brain, such as the tract connecting the amygdala, a small region involved in emotional processing and memory formation, and the subgenual anterior cingulated cortex (sgACC), which is vital in regulating amygdala responses. This connection, the uncinate fasciculus, has an important role in certain psychiatric illnesses. To compare the conventional deterministic algorithm and our message passing-based algorithm, we wanted to focus on determining the location of this connection within the brain.

Two images were taken: one high-resolution macaque brain image and one low-resolution human brain image using a 7T Bruker BioSpin magnetic resonance system and a Siemens 3T Trio scanner respectively. The deterministic and probabilistic approach was then tested using the images.
Using the probabilistic message passing algorithm, we were able to clearly trace the fibers in the high resolution macaque data (Figure 1). The deterministic approach was also able to locate the fibers in this data. However, in the low resolution data of the human brain, the deterministic approach failed to locate the uncinate fasciculus, while the probabilistic approach clearly located the uncinate fasiculus (Figure 2).

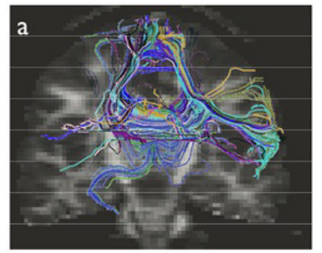

Figure 4. Visualizations of the connective fiber tracts throughout the low-resolution human brain. (a) A coronal view of fibers using the deterministic approach. (b) A coronal view of fibers calculated using the message passing algorithm.

"In the low resolution data of the human brain, the deterministic approach failed to locate the uncinate fasciculus; however, the probabilistic approach clearly located the uncinate fasiculus."

"Once validated, however, this approach can be a useful tool for future fiber tract studies."

A New Approach

This probabilistic message passing-based algorithm was able to locate the uncinate fasciculus with high detail in comparison to the deterministic algorithm. Our data shows that the uncinate fasciculus does not directly connect the amygdala to the anterior cingulated cortex as predicted, but that there may be an indirect connection. Further research is needed to verify the possible fiber connections. In addition, we found that our probabilistic message passing algorithm is more precise than the deterministic approach. We were able to locate more fibers that, on average, had a longer length. However, these results should be compared to known fiber tracts to ensure their accuracy. Once validated, however, this approach can be a useful tool for future efficient fiber tract studies.

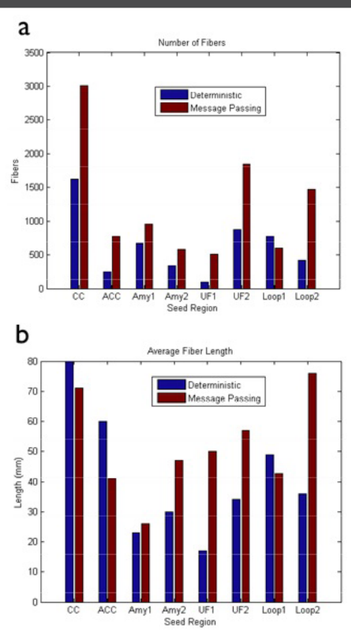

Figure 5. A quantitative comparison between the deterministic and message passing-based algorithm results for the low-resolution human brain data (Figure 4). (a) The number of fibers located in each region using the deterministic approach and the message passing-based approach marked in blue and red respectively. (b) The average fiber length located in each region using the deterministic approach and the message passing-based approach marked in blue and red respectively.

Acknowledgements

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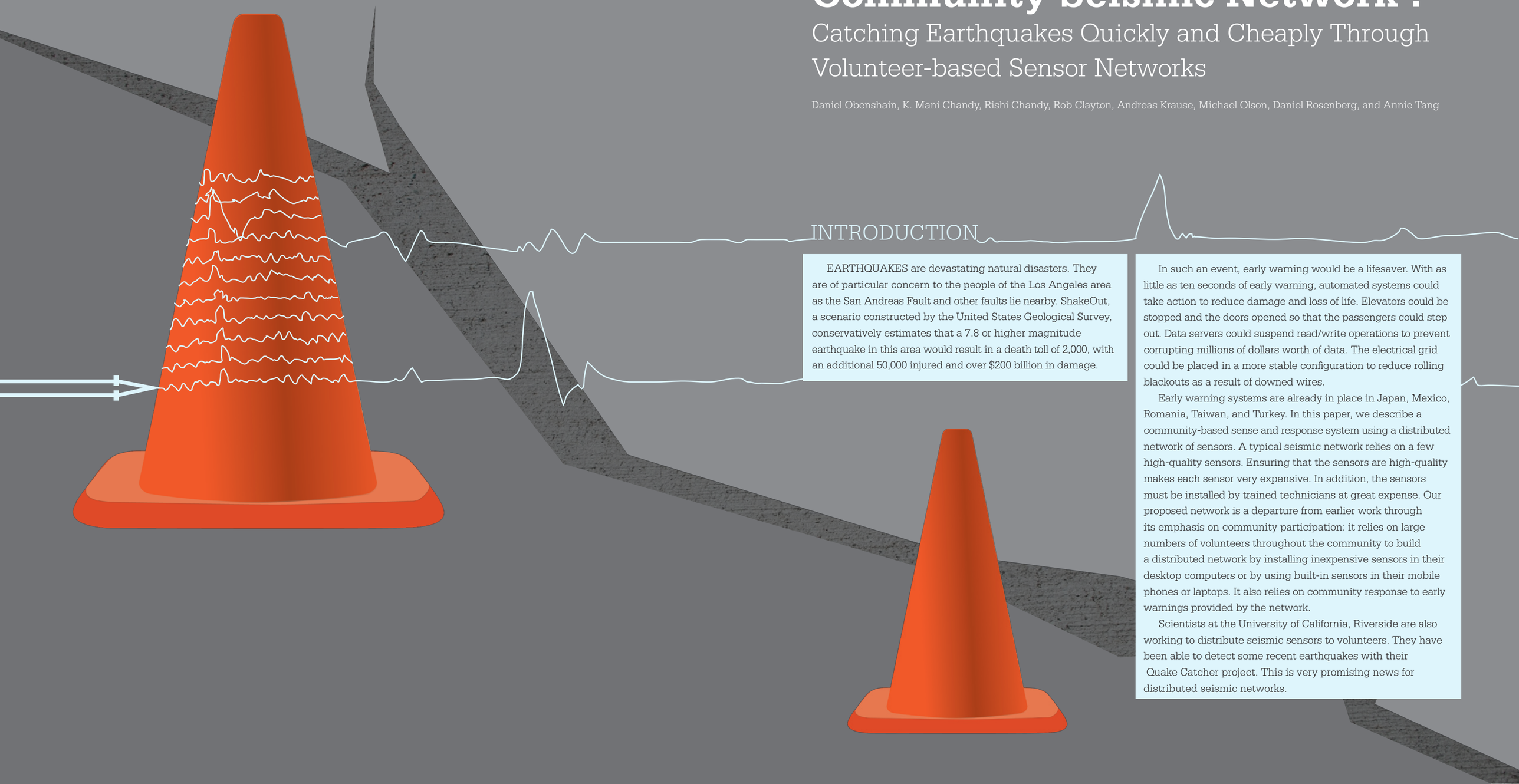
Community Seismic Network :

Catching Earthquakes Quickly and Cheaply Through Volunteer-based Sensor Networks

Daniel Obenshain, K. Mani Chandy, Rishi Chandy, Rob Clayton, Andreas Krause, Michael Olson, Daniel Rosenberg, and Annie Tang



INTRODUCTION

EARTHQUAKES are devastating natural disasters. They are of particular concern to the people of the Los Angeles area as the San Andreas Fault and other faults lie nearby. ShakeOut, a scenario constructed by the United States Geological Survey, conservatively estimates that a 7.8 or higher magnitude earthquake in this area would result in a death toll of 2,000, with an additional 50,000 injured and over $200 billion in damage.

In such an event, early warning would be a lifesaver. With as little as ten seconds of early warning, automated systems could take action to reduce damage and loss of life. Elevators could be stopped and the doors opened so that the passengers could step out. Data servers could suspend read/write operations to prevent corrupting millions of dollars worth of data. The electrical grid could be placed in a more stable configuration to reduce rolling blackouts as a result of downed wires.

Early warning systems are already in place in Japan, Mexico, Romania, Taiwan, and Turkey. In this paper, we describe a community-based sense and response system using a distributed network of sensors. A typical seismic network relies on a few high-quality sensors. Ensuring that the sensors are high-quality makes each sensor very expensive. In addition, the sensors must be installed by trained technicians at great expense. Our proposed network is a departure from earlier work through its emphasis on community participation: it relies on large numbers of volunteers throughout the community to build a distributed network by installing inexpensive sensors in their desktop computers or by using built-in sensors in their mobile phones or laptops. It also relies on community response to early warnings provided by the network.

Scientists at the University of California, Riverside are also working to distribute seismic sensors to volunteers. They have been able to detect some recent earthquakes with their Quake Catcher project. This is very promising news for distributed seismic networks.

HOW THE SYSTEM WORKS

Under our system, a volunteer will be able to use one of several different kinds of accelerometers to make his or her computer a client in our network. Each client will then log seismic data using the accelerometer. If significant shaking occurs, the client computer will "pick" that data and send a message to the server, alerting it to possible earthquake activity.

The server will receive a stream of picks from clients scattered throughout the Los Angeles area. It will then evaluate the incoming picks to determine if it is likely that an earthquake is currently occurring and, if so, where. The server will then immediately generate a ShakeMap, which will be very useful for evaluating damage and organizing relief efforts. An early version of this can be seen in (Figure 1). Ideally, an estimate of the size and location of the earthquake will be generated before the bulk of the shaking actually occurs, allowing the system to distribute that information in the form of an early warning.

The data-picks stream will inevitably contain a lot of noise. Since these sensors will not be underground or connected to bedrock, they will be subject to vibrations in their environments. It is reasonable to assume that users will often accidentally set off their sensors by bumping them or kicking the table on which the phone or laptop rests. It is therefore important to have a dense network so that noise will be dampened by the information from the surrounding network.

Since this network needs to be very trustworthy, we have included an additional playback feature. If requested, the server can distribute prerecorded acceleration data to the clients. At a specified start time, the clients would play back the data to simulate an event across the entire network. This feature will allow us to effectively test the system, checking the ability of clients to provide accurate reporting of earthquake events as well as simulating historical events (such as the 1994 Northridge quake) to determine how our system would have reacted to an actual natural disaster. Successful testing will greatly increase public confidence in our system and encourage widespread participation.

Fig. 1. Screenshot of the web interface showing simulated shaking detected by sensors around Caltech.

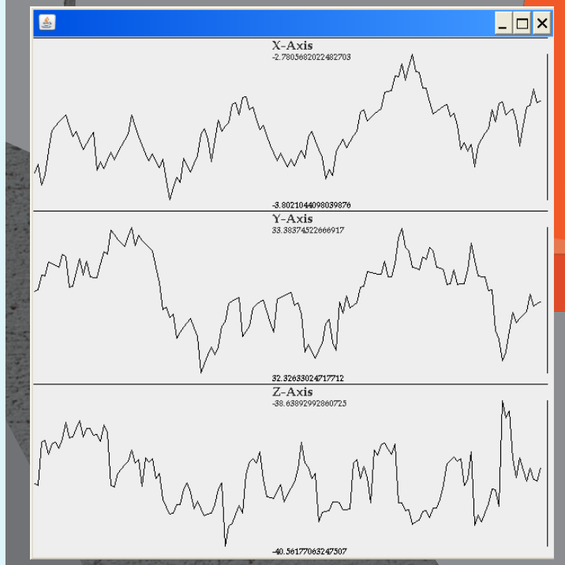


Fig. 2. The user is able to see the data gathered by his or her computer.

SYSTEM DESIGN

Conceptual

This network of sensors will rely on Internet communications and volunteer support from the public. Each participating individual will use an existing accelerometer device inside his or her computer or mobile phone or purchase an accelerometer device and connect that device to his or her computer (see figures 4 and 5 for a prototype of such a device). The participant will then download and execute software from our server to begin sending data. Once the data is received by the server, the server will be able to use that information for early warning.

Client

Once the client computer has downloaded and installed the necessary software, it will be part of our seismic network. Whenever the client computer is free, it will read data as often as possible from the accelerometer and store it in a buffer on the client's computer. The data is processed with an exponential filter to reduce noise. The frequency of data is limited by the hardware used; for the example client shown in Figure 2 it is approximately 60 data points per second. The buffer will be read by a picking algorithm, which will trigger and send a message to the server if seismic activity is suspected. The picking algorithm is described later in the paper. In order to minimize inconvenience to participants, the whole application will run silently in the background and require minimal system resources.

To encourage use, participants will be able to watch the data stream gathered by his or her machine in real-time via a graphical user interface (Figure 2).

In addition to these features, the client will be able to "play back" a simulated dataset. Once a day, the client will "call home" to alert the server to its presence. To assure participants of their privacy and security, the server will never be allowed to initiate contact with the client. After receiving the initial message, the server will alert the client to any playback requests. If the client receives a playback request, it will create a new thread which will activate at a specified start time. The new thread will then start reading data from the file given by the server, rather than the accelerometer. This will allow us to test the network from end to end as previously described.

Server Architecture

The server will collect all the pick data sent by the clients. It will then use existing Associator and Locator code to pinpoint the earthquake event. The Associator will associate a group of picks with a seismic event, which will then allow the Locator to locate the epicenter of that event. The server will use this data to output a ShakeMap, a heat map that uses different colors to provide an easily interpretable graphical display of shaking intensity (see Figure 1). This will aid in early warning and relief efforts.

Picker

Ideally, the algorithm will "pick" acceleration data only if seismic activity is present. In practice, such accuracy is not always possible; instead, the algorithm will "pick" whenever there is a sufficiently large change in the acceleration detected by the client. By properly calibrating the "picking" threshold, we attempt to maximize the probability of picking up true seismic events while minimizing the probability of false positives due to, for example, jostling of the sensor.

The picking algorithm depends on a comparison of short-term and long-term averages of recently recorded accelerations. The number of data points aggregated is variable, but currently the short term average aggregates the most recent ten data points, while the long term average aggregates the most recent 250 data points (for our example client, this is a little more than 4 seconds). If the ratio of the short-term to long-term averages exceeds a threshold value (for example, 10 percent above the long term average), the client assumes that a seismic event is occurring and "picks" that data. The threshold value is variable to account for different sensor conditions for different clients - for example, some clients, such as mobile phones, may be more prone to random jostling than others, like laptops.

Once the picking algorithm has triggered, the software immediately saves the contents of the buffer to the hard drive on the assumption that the computer might soon lose power. This feature assures that if the accelerometer is attached to a desktop computer with no backup power source, recorded data will not be lost if an earthquake knocks out power, and will be available for later analysis once power is restored.

The software then continues recording data for a short time t_{pause} to determine as accurately as possible the magnitude of the shaking.

Finally, the software sends the "picked" data to the server for association. Some time later, the software saves the buffer to the hard drive again to ensure that the entire earthquake was captured. Finally, the client waits some time t_{delay} before picking earthquake and falsely reporting multiple earthquakes when in reality only one has occurred.

Both t_{pause} and t_{delay} are parameters that can be tuned,both throughout the network and at the level of the individual client. If t_{pause} is too long, the shaking information will not reach the server in time and the server will not be able to give an effective early warning. On the other hand, if t_{pause} is too short, the client will underestimate the magnitude of the shaking, resulting in incorrect estimates of the earthquake's magnitude. If t_{delay} is too short, the client will send several messages to the server for the same set of shaking, which will bog down the server and produce false reports of multiple back-to-back quakes. If t_{delay} is too long, the client might miss a second earthquake occurring soon after the first one, failing to report ACTUAL back-to-back quakes! The server will be able to calibrate these values on the client's computer during the daily synchronization period to maximize the network's accuracy and effectiveness.

Associator

The server receives a constant stream of data from the clients and the clients "pick" data. An Associator program on the server associates the incoming data with existing data to determine if it is likely that an earthquake has just occurred.

If such an earthquake is likely, the server estimates the likely epicenter and intensity of the earthquake and passes on this information to emergency services and other early-response systems. Ideally, this information could then be distributed before significant shaking had occurred.

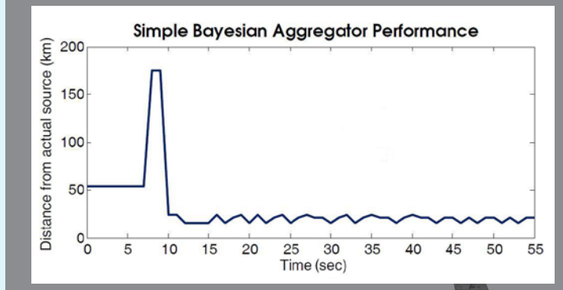


Fig. 3. Results obtained by running the simple Bayesian aggregator on synthetic pick data. The x-axis represents the number of seconds since the the earthquake and the y-axis represents the difference between the estimated epicenter and the actual epicenter. The spike represents an early error in the estimation due to erroneous data.

The simple aggregator developed by Andreas Krause uses Bayesian inference to locate the source of an earthquake. Bayesian inference begins with a "guess" or "prior" probability distribution giving the probability of an earthquake of a given magnitude occurring at a particular place and time. (For example, this distribution might be drawn from historical data.) As pick data is gathered, the algorithm updates the distribution of earthquake probabilities by determining the likelihood of the picks data given particular earthquake parameters. In essence, earthquake parameters that were more likely to have generated the picks data are "promoted" and given higher probability in the updated distribution; but how much they are promoted depends on how likely we expected those parameters to be in the first place. Over time, updating the probability distribution with picks data should produce a distribution sharply peaked at the true earthquake magnitude, location, and time. The prior distribution we used is based on the Gutenberg-Richter Law, which gives a relation between an earthquake magnitude and the expected number of earthquakes in a region that were of at least that magnitude. The likelihood function is based on a normal distribution of pick arrival times.

The aggregator was tested using synthetic pick data, with performance shown in (Figure 3). As can be seen in the figure, in this simulation we determined the origin of the earthquake to within 25 km after approximately 10 seconds. The sythentic pick data included some erroneous picks to make the simulation more realistic, which caused the early spike in the error. We are currently implementing this portion of the system on Google App Engine. This gives us the advantage of using Google's distributed server network. It is unlikely that a single earthquake would simultaneously take down all of Google's servers, giving us a robust platform with which to host the associator software.

Machine Learning

Each client has many parameters associated with it: t_{pause}, t_{delay}, the number of data points in the short term average, the number of data points in the long term average, and parameters associated with the signal filters. In order to improve the network, we can tune these parameters on a client by client basis. For example, if a client is located next to a construction site with a jackhammer, that client's data is not very useful for low levels of shaking, since those levels of shaking are indistinguishable from the shaking caused by the jackhammer. We can improve the reliability of the network by raising that client's threshold to decrease the number of false positives. Once fully implemented, the server will be able to detect excessive false positives and alter the parameters dynamically to maximize network accuracy.

We expect the optimal parameters generated by the machine learning algorithm to reflect underlying physical events. For example, we expect t_{pause} to be about the duration of the first shock of an earthquake (approximately 1 second).

EVALUATION

Since it is vitally important to establish the reliability of our sensors, we compared a sensor's performance against an existing high-quality sensor in the Southern California Seismic Network (SCSN).

Our sensor consisted of a Phidget brand accelerometer (approximately $90) connected to an Eee PC (approximately $300). The low cost of this setup (particularly considering the high rate of existing computer ownership by the community) is one of the strengths of our system; for an insignificant cost compared to current systems, a robust network of distributed sensors can be rolled out community-wide to detect potential earthquakes.

We set up our sensor in the basement of Millikan Library on Caltech's campus, next to a conventional sensor designated MIKB for its location in Millikan Basement (Figure 6). Both devices were placed in a small basement maintenance room (Figure 7). After simulating an earthquake by hitting the concrete floor with a sledgehammer, we compared the waveforms received by both devices (Figure 8).

While the data gathered by our example sensor had much more noise than the conventional sensor, both detected acceleration spikes at the same times. As is readily apparent, the signal-to-noise ratio of our sensor is quite poor (less than 14 dB, or a peak-to-noise amplitude of about 5-to-1). We expect that by implementing improved signal filters, we will substantially improve the signal-to-noise ratio and produce clearly defined acceleration spikes that will be readily detected by the "picking" algorithm.

Some of the noise in our sensor's data is random noise. This is a necessary trade-off of using low-cost sensors. However, the use of a distributed network of many sensors will wipe out this noise. Because random noise is uncorrelated across sensors, and because the data from many sensors will be averaged in the Associator, random noise will be damped out and won't interfere with earthquake detection.

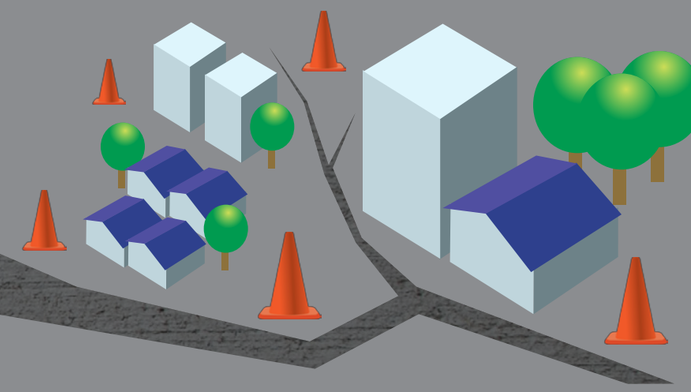


Fig. 4. The accelerometer device, before it has been connected to a computer.

Fig. 5. An example client. The accelerometer device is seen here connected to the USB port on an example laptop.

Fig. 6. Sensor MIKB. This is one of the sensors in the Southern California Seismic Network, and is designated MIKB since its location is in the basement of Millikan Library on the Caltech campus.

Fig. 7. The arrangement of the two sensors. Both the example client and the MIKB sensor are visible. Also seen here is the sledgehammer used to simulate seismic activity for testing purposes.

FUTURE DIRECTIONS

Our work demonstrates the possibility of inexpensive and effective early-warning systems to reduce the costs of future earthquakes. By using a system of cheap sensors, we reduce the necessity of installing multi-million dollar high-quality senor arrays to monitor seismic activity. By basing detection on a distributed community-based network of sensors, we ensure robust, reliable data collection and estimation of earthquake locations and intensities.

The next steps in implementing the Community Seismic Network will be encouraging widespread participation and establishing distribution channels for the information gathered by the system. We are confident that the low cost of the system (in fact zero cost to owners of cell phones or laptops with builtin accelerometers) combined with the inherent "coolness" of knowing that one's computer is collecting seismic data will ensure adequate participation in the system. Our simulated playback feature will also demonstrate the network's power and effectiveness, which combined with sufficient publicity of results should encourage even more members of the community to buy into the idea.

Distributing the information to early-responders will be more challenging, as many systems (e.g. elevators, electrical grids) will require retrofitting to take advantage of the data provided by the Community Seismic Network. Nonetheless, the huge net cost savings of implementing an effective early warning system instead of merely waiting passively for an earthquake to happen should motivate implementation of such changes.

Scientists still can't reliably predict earthquakes; but we DO have the capability to detect them in their early stages and take preventative action to limit the destruction they cause. The Community Seismic Network seeks to make this idea an affordable reality.

Fig. 8. The impact of the sledgehammer, as detected by the two sensors. The signal detected by our sensor is much less clean.

ACKNOWLEDGMENTS

We would like to thank Dr. Carol Readhead, Eric Chin, and Erik Madsen for proofreading this manuscript.

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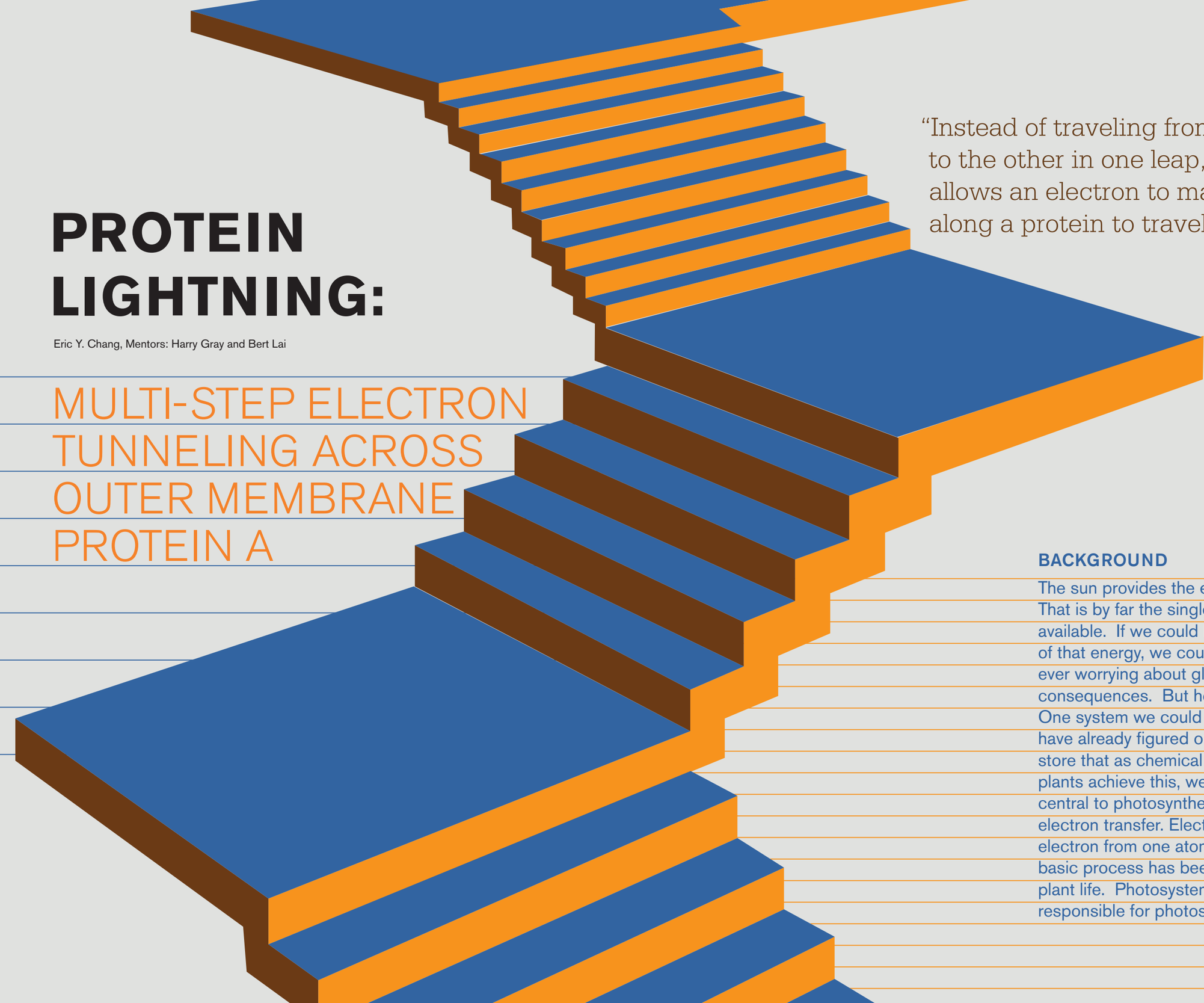
PROTEIN LIGHTNING:

Eric Y. Chang, Mentors: Harry Gray and Bert Lai

MULTI-STEP ELECTRON TUNNELING ACROSS OUTER MEMBRANE PROTEIN A



"Instead of traveling from one end of a protein to the other in one leap, multi-step tunneling allows an electron to make smaller jumps along a protein to travel the same distance."

BACKGROUND

The sun provides the earth with 1.2 x 10^5 TW of power. That is by far the single largest source of clean energy available. If we could harvest even a fraction of a percent of that energy, we could power the planet forever without ever worrying about global warming or other environmental consequences. But how do we collect solar power? One system we could look to is photosynthesis. Plants have already figured out how to collect solar energy and store that as chemical fuel. In order to understand how plants achieve this, we must examine the phenomena central to photosynthesis–a lightning fast reaction called electron transfer. Electron transfer is the movement of an electron from one atom or molecule to another. This basic process has been perfected in nature to sustain plant life. Photosystem II, a large protein complex responsible for photosynthesis, is incredibly efficient,

transferring an electron over 50 Å in picoseconds. The exact mechanism of this process, though, is still a mystery. Attempts to replicate an electron transfer reaction in vitro have shown that electrons traveling even 20 Å across a model protein take at least a millisecond (Figure 1); this electron transfer speed is too slow to support life. One way that plants might speed up the rate of electron transfer across a protein is with multi-step electron tunneling. Instead of traveling from one end of a protein to the other in one leap, multi-step tunneling allows an electron to make smaller jumps along a protein to travel the same distance. The difference between these two methods of travel can be compared to climbing a one-step staircase spanning two floors as opposed to a staircase with five or six steps, which would be easier to climb. By lowering the energy required for each jump, multi-step tunneling increases the probability that an electron will be able to travel across a protein, thereby increasing the rate of transfer. Recently, the Gray Group has engineered a modified bacterial amino acid that performs a two-step electron transfer. In this model, electrons travel 19 Å across a two-step pathway two orders of magnitude faster than the speed of an electron in a single-step electron transfer (Figure 1).

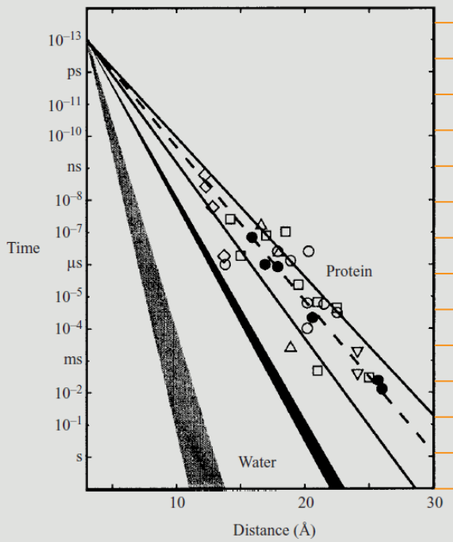


Figure 1 / Timetable for single-step electron tunneling in Ru-modified metalloproteins.

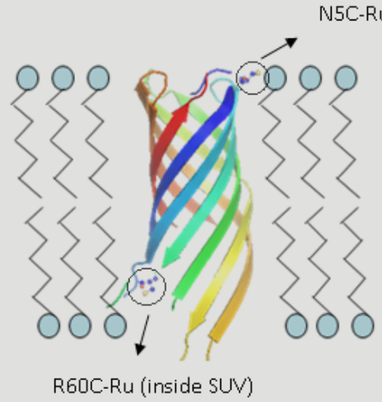


Figure 2 / Schematic of mutation locations and covalently linked labels

"These results verify that N5C-Ru and R60C-Ru were folding correctly."

Omping Up Electron Transfer

In order to extend these results to more complex reactions, we have examined multi-step electron tunneling to hypothetically mimic Photosystem II. Because Photosystem II is a very large and complicated protein, a simpler protein was chosen for modeling from the cell membranes of E. coli cells, namely the outer membrane protein A (OmpA). OmpA is composed of an eight-stranded ββ-sheet that induces fast electron transfer rates similar to Photosystem II, making it an ideal model protein. To study electron transfer in OmpA, we introduced cysteine (C) amino acid mutations at position 5 and 60 in the protein because they allow us to covalently link Ru(II)(iodoacetamide-phen)(bpy)2 and Re(I)(iodoacetamide-phen)(CO)3(im)—which are electron donor and acceptor ruthenium metal complexes functioning as labels to help us measure speed of electron transfer—to these sites. Figure 2 shows the locations of the C mutants. The distance between the electron donor and acceptor is approximated to be 38 Å, which will take seconds for an electron to traverse in a single step electron transfer process. However, it is hypothesized that the multi-step electron transfer in this tryptophan mediated system should be much faster. Tryptophan is an amino acid that readily transfers electrons, and thus can act as one of the intermediate steps in a multi-step transfer.

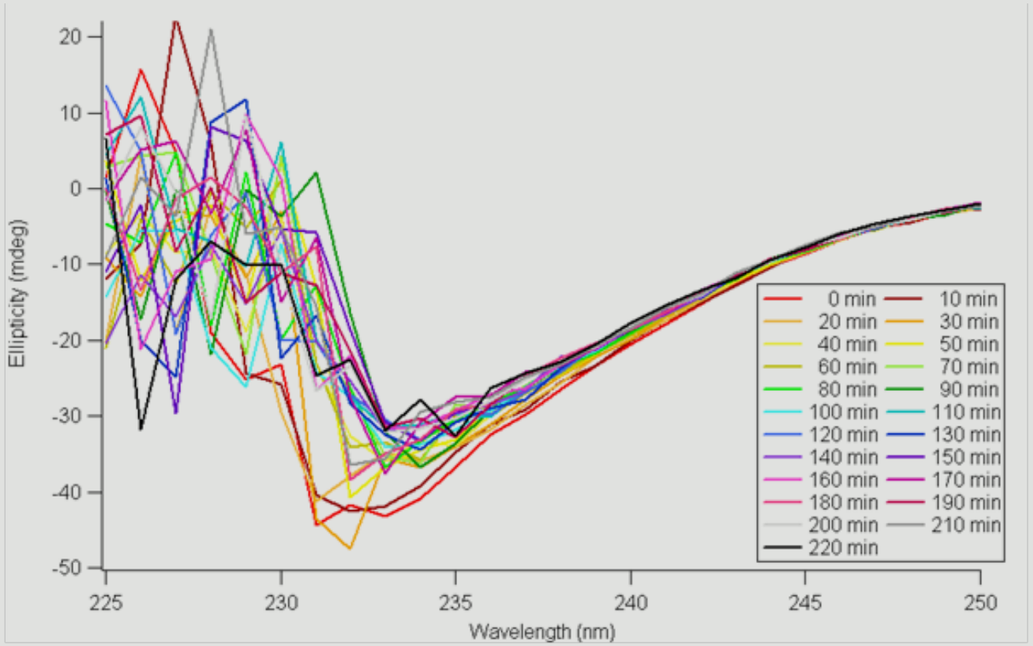


Fig 3 / R60C-Ru in SUV (CD)

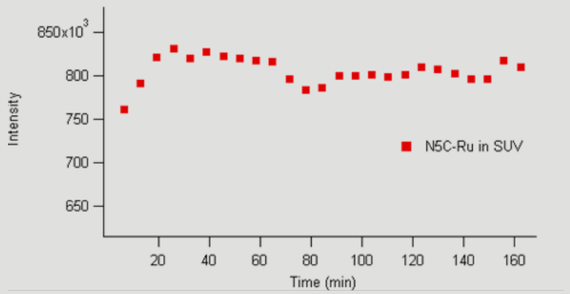


Figure 4 / R60C-Ru in SUV

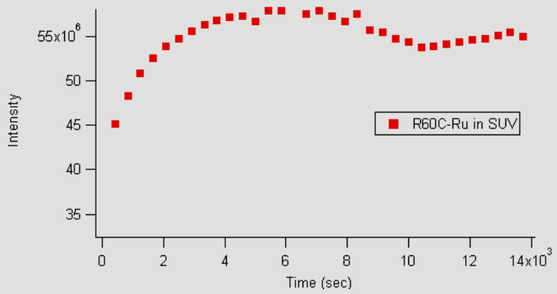


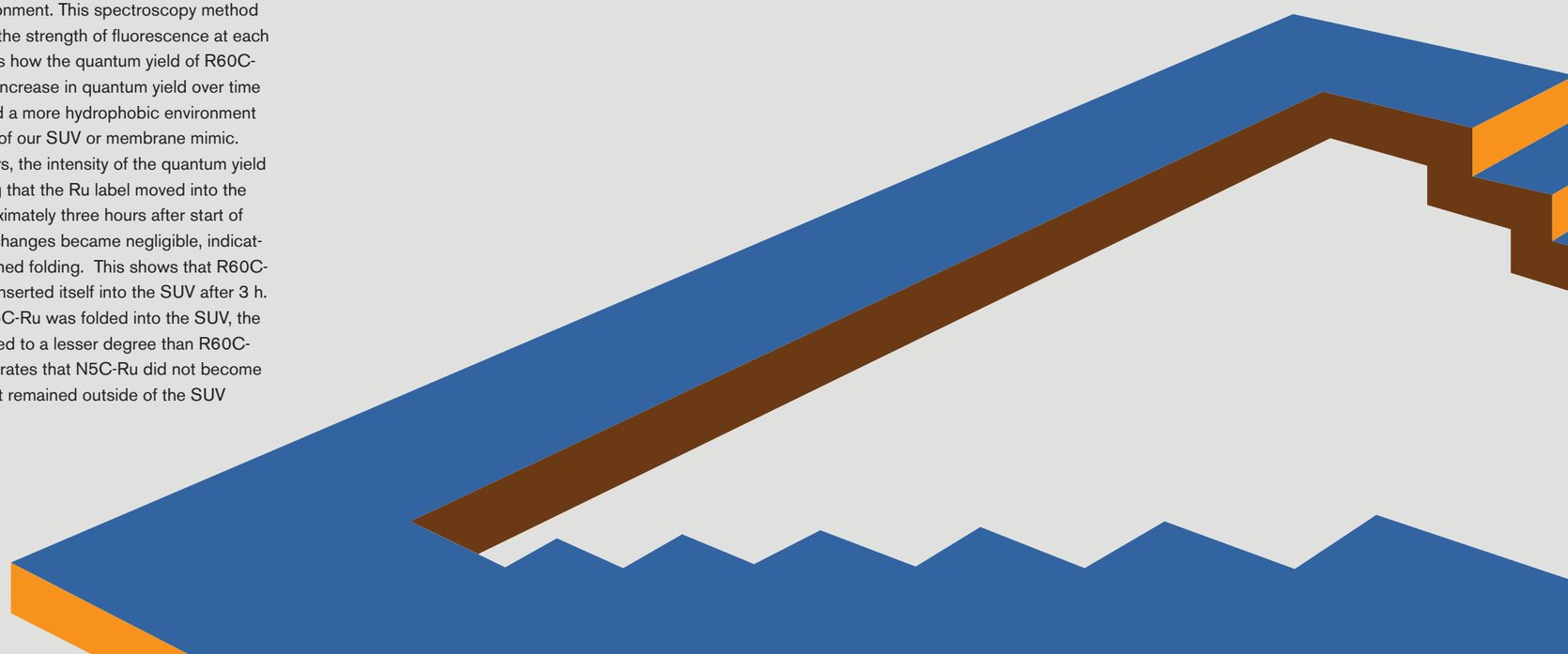
Fig 5 / N5C-Ru in SUV

Before electron transfer could be assessed, we needed to determine whether the modified OmpA protein will still fold correctly when labeled with the ruthenium metal complexes. After covalently binding the ruthenium metal complexes to the cysteine amino acids at positions 5 (N5C-Ru) and 60 (R60C-Ru), the protein was folded into cell membrane mimics, or small unilammellar vesicles (SUVs). By labeling at two different locations, we could more accurately predict whether our protein is folding correctly. Steady state fluorescence and circular dichroism studies, which are different methods of shining light at the protein to gather information about structure, were performed to spectroscopically determine whether OmpA folds correctly when labeled with the ruthenium metal complexes.

Circular dichroism was first used to determine whether the two different R60C-Ru- and N5C-Ru-labeled protein regions folded correctly into the appropriate ß-barrel shape. We can see in Figure 3 that the classic indicator for ß-sheets, a checkmark-like shape over the 230 nm to 245nm range, is present. This study demonstrated that our ruthenium labeled OmpA protein was folding properly in terms of secondary structure.

Steady-state fluorescence was then conducted on the modified OmpA to determine whether the two fluorescence labels have folded into the correct environment. This spectroscopy method measures quantum yield, or the strength of fluorescence at each label. Figure 4 demonstrates how the quantum yield of R60C-Ru changes over time. The increase in quantum yield over time indicates that the Ru entered a more hydrophobic environment corresponding to the inside of our SUV or membrane mimic. After approximately two hours, the intensity of the quantum yield decreases slightly, indicating that the Ru label moved into the cavity of the SUV. By approximately three hours after start of spectroscopy, the intensity changes became negligible, indicating that the protein had finished folding. This shows that R60C-Ru successfully folded and inserted itself into the SUV after 3 h. On the other hand, when N5C-Ru was folded into the SUV, the quantum yield initially changed to a lesser degree than R60C-Ru (Figure 5). This demonstrates that N5C-Ru did not become embedded within the SUV; it remained outside of the SUV as we expected.

“Electron transfer is the movement of an electron from one atom or molecule to another. This basic process has been perfected in nature to sustain plant life.”



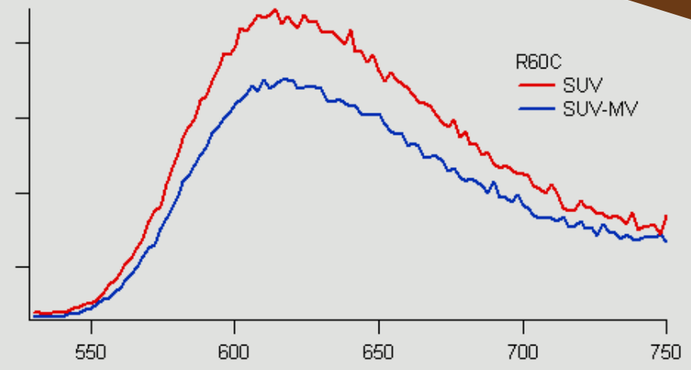


Figure 6 / MV Encapsulated in SUV: N5C-Ru

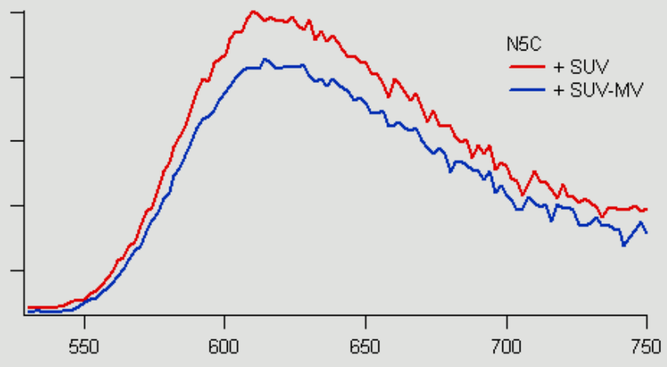


Figure 7 / MV Encapsulated in SUV: R60C-Ru

"Using our model protein, we can begin to eventually study the kinetics of our multi-step tunneling electron transfer process in proteins."

At this point we believed our modified OmpA protein labeled with Ruthenium was folding correctly into both its ß-barrel structures and position in a membrane. As a further check, however, we performed quenching experiments. A quenching experiment allows us to measure how close each metal complex label is to the quencher, which we can place either inside or outside of the SUV. Figures 6 and 7 document the effects of adding a methyl viologen quencher, encapsulated inside the SUV, on the fluorescence of Ruthenium. With the quencher added, the R60C-Ru experienced a larger drop in quantum yield, or fluorescence, than N5C-Ru, indicating that R60C-Ru was in closer proximity to the quencher located inside the SUV. The experiment was repeated with the methyl viologen quencher added to the outside of the SUV. In this case, the N5C-Ru experienced a larger drop in quantum yield, demonstrating that N5C-Ru and the quencher interacted more closely, thereby confirming that the N5C-Ru was located outside the SUV. These results further verify that N5C-Ru and R60C-Ru were folding correctly.

LOOKING TO THE FUTURE

Having confirmed that the modified OmpA labeled with ruthenium metal complexes folds correctly, we have laid the foundation for studying electron transfer reactions across membranes in the OmpA system. Using our model protein, we can begin to eventually study the kinetics of our multi-step tunneling electron transfer process in proteins. The long term goal of this project is to see how we can speed up the electron transfer process by adding tryptophan amino acids throughout the protein. Eventually, by understanding the extremely fast process of electron transfer across membranes, we might be able to replicate these reactions to generate clean energy from the Sun.

Acknowledgements

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