

the

THE UNIVERSITY OF  
TEXAS AT DALLAS  
UNDERGRADUATE  
RESEARCH JOURNAL

# Exley

VOLUME 1 SPRING 2012

*Inaugural Issue*

*Featuring*

**An Interactive Toolbox for the Analysis of  
Volcanoes on Earth and Mars**

*Emily Butler*

**Social Media Return on Investment:  
Tracking and Measurement**

*Zachary Johnson*

**Antimicrobial Activity of Plant Extracts:  
How Common Vegetables and Oils Can Change  
the Way Diseases Are Treated**

*Syed Muhammed Rasheed*

# About The Exley

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Dear Readers,

The articles and creative works published in *The Exley* showcase the hard work and dedication of the student authors and their faculty mentors. I hope these works inspire other students to become engaged in research and share their creative work with our university community through *The Exley*.

UT Dallas values the undergraduate research experience and encourages its students, regardless of discipline, to seek out and participate in the creation of knowledge. UT Dallas undergraduate students are engaged in research activities with our nationally recognized faculty and post-doctoral fellows. *The Exley* was established to provide a platform for UT Dallas undergraduates to publish research articles and creative works.

The works published in *The Exley* reflect the valuable and enriching experiences UT Dallas provides students and the impact of faculty research on undergraduate education. *The Exley* is managed by the Office of Undergraduate Education and is produced in collaboration with staff, administrators from each school, faculty, and students.

In closing, I would like to personally thank Ms. Elizabeth Exley Hodge, who dedicated nineteen years to UT Dallas as an employee. Her generous support helped found this journal. *The Exley* is named in her honor. The Office of Undergraduate Education recognizes her generosity and commitment to continued excellence in undergraduate research.

Sincerely,

A handwritten signature in blue ink, consisting of a stylized, cursive name that ends in a long horizontal line.

Sheila Amin Gutiérrez de Piñeres, PhD  
Dean of Undergraduate Education

# Our Name

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In the Spring of 2011, Ms. Elizabeth Exley Hodge made a generous donation to support the publication of UT Dallas' first interdisciplinary undergraduate research journal. Hodge's maiden name Exley represents the rich history of her family. Her brother, John, searched records in Manchester and Halifax, England in 1971, which revealed that the surname Exley was believed first to be Ecclesley, dating from 1245, meaning "Church Fields." The area where her great-great-grandfather was born now exists as Exley Hall in Yorkshire, England. Several in the current family have visited there. The journal was named *The Exley* to show the university's appreciation of Hodge's support.

## **Elizabeth Exley Hodge Biography**

Hodge was born in a small farming community in Worcester County, Maryland, in 1920. She is one of eleven children of Lola Marie Watson and John O. Exley, who had distinguished himself with gold medals in rowing at the 1900 and 1904 Olympic Games. After high school, Hodge lived nine years in Philadelphia, where she worked for an insurance company. When World War II was declared, she volunteered in a program with the U.S. Air Corps, where she met the man she later married, Noble H. Hodge, from Fannin County, Texas. They were married in 1942. Following his military service in England, they moved in 1945 to Dallas, Texas, where Hodge still resides. In 1967, Hodge joined the administrative offices of the Southwest Center for Advanced Studies. When the center became UT Dallas in 1969, she transferred to the Department of Biology in the School of Natural Sciences and Mathematics, where she assisted faculty members preparing research grant applications. After a number of years in grants management in the School of Natural Sciences and Mathematics and later in the Office of Sponsored Projects, she retired in 1986. Hodge has been an avid gardener for many years. She has a personal arboretum and an orchid hybrid that bears her name. She enjoys cooking and sharing her time with others. Hodge has volunteered weekly for the last 23 years at Baylor Medical Center in Garland. She is a member of St. John's Episcopal Church near her home.

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# ABOUT the Contributors

## Micheal Ansley

from Royse City, Texas, is a junior majoring in computer science. Ansley, who has Asperger's syndrome, has found photography to be a rewarding way of sharing the logic and mathematics he finds prevalent in both nature and man-made objects of the every day world that surrounds us all. Photography has also enabled Ansley to develop a comfortable level of communication with others that often offsets the social difficulties caused by his Asperger's, thus affording him the ability to participate in a more well-rounded campus experience.



## Syed Muhammed Rasheed

is a junior psychology and child learning & development double major from Carrollton, Texas. Rasheed's article is based on work he did with The Center for Advanced Studies in Mathematics and Natural Sciences (CASMS). His passion for research in microbiology started when he began working with Dr. Sukanya Subramanian in his sophomore year of college. He enjoyed trying to figure out which groups of plant products work best in killing different kinds of bacteria. Rasheed says that his research can help people understand the importance of eating organic foods and also educate them on natural ways of fighting illnesses. In addition to his interest in microbiology, Rasheed is also interested in learning and researching autism. Currently, Rasheed is working in Dr. Noah Sasson's social cognition lab as a research assistant where he is involved in autism research. Although busy with his academic studies, Rasheed also finds time for his passion for sports. He enjoys playing and watching basketball, tennis, and football with his friends. After graduation, Rasheed plans to attend medical school and pursue a career in pediatric neurosurgery.

**Honors:** Brain and Behavioral Sciences Honors Program and Honor Society of Alpha Epsilon Delta.



## Matthew McCann

is a junior electrical engineering major from Port Isabel, Texas. His project was an expansion of the 2011 International Future Energy Challenge proposal. After graduating, McCann hopes to obtain a master's degree in business administration and PhD in electrical engineering, and he would eventually like to teach at the collegiate level. He is grateful to his faculty advisor, Dr. Babak Fahimi, for encouraging him and supporting his research.



## Larissa Weidenbruch

is a senior literary studies major with teacher certification in English Language Arts and Reading for grades 4-8. She first became interested in an academic approach to LOLcats during a linguistics class. The project began as a linguistic analysis of the LOLspeak language and expanded to a thesis with a focus on fandom after Weidenbruch took a class on American popular culture. She plans to pursue a master's degree in literature and to become a teacher.

**Honors:** Collegium V Honors, School of Arts and Humanities Honors, Summa Cum Laude Graduate, Phi Kappa Phi Honor Society, Delta Epsilon Iota Honor Society, Dean's List, Academic Excellence Scholarship.



**About the Contributors**

# Emily Butler

is a senior geophysics major and mathematics minor from Plano, Texas. Her toolbox aims to simplify research associated with volcanoes on Earth and Mars by combining databases and visual imaging techniques. She hopes that this toolbox will show insight to the history of Earth and Mars and perhaps provide information on other possible life-sustaining exoplanets. After graduating, she plans to attend graduate school for a master's degree in geophysics.



# Linda Wilson

is a senior neuroscience major, with a minor in psychology. She is a member of Psi Chi International Honor Society and Tau Sigma National Honor Society. She enjoys creative arts, including photography, in her spare time. Wilson has been working in a neural engineering lab on campus for the past two years and plans on attending graduate school to pursue a career in neuroscience research.

## About the Contributors





## Truc K. Do

is a junior biochemistry major from Allen, Texas. She researched slime molds in Dr. Dennis Miller's lab at UT Dallas and spent her summers assembling the genome of flu viruses at Los Alamos National Laboratory. Her interest in genetics became a passion, one that she communicated with fellow students as a teaching assistant. Currently, she is studying the genetics of obesity at UT Southwestern (UTSW). She plans to obtain a doctorate in molecular genetics and microbiology to prepare for a career in academia and research.

**Honors:** Eugene McDermott Scholars Program, 2011 Barry M. Goldwater Scholarship Honorable Mention, Green Fellowship at UTSW, Phi Kappa Phi Honor Society, and Collegium V Honors Program.

## About the Contributors



## Jessie Gonzales

is a senior electrical engineer major from McKinney, Texas. Gonzales' article is based on research he and PhD student, Connie Manz, conducted last summer under the guidance of Dr. Walter Voit. What attracted him to participate in the summer research were the interesting behavior of acoustic metamaterials and the opportunity of fabricating a new, innovative class of acoustic metamaterials with extensive features. Encouraged by Dr. Voit to share his research findings with a broad audience, Gonzales decided to write for the newly formed undergraduate journal. He plans on attending graduate school next fall for a master's of science in electrical engineering.

## Triet S. Nguyen

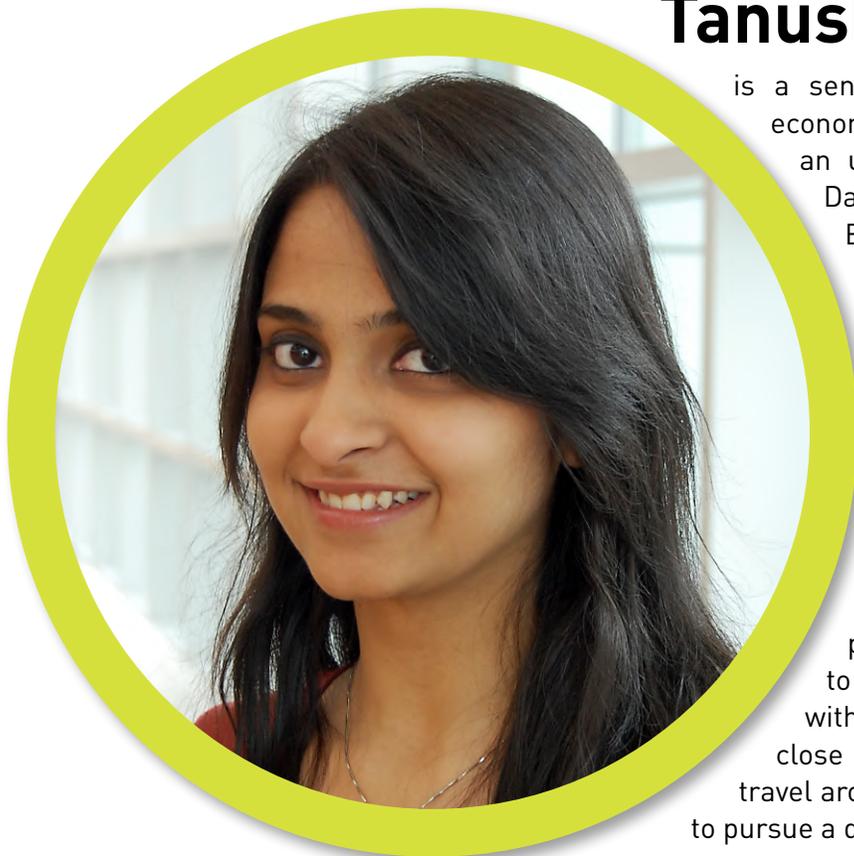
is a senior biochemistry major originally from Saigon, Vietnam. Introduced to computational chemistry by her professor, Dr. Steven Nielsen, she has since been involved in research on molecular dynamic simulations. With an interest in medical applications of computational chemistry, she plans to attend graduate school and pursue a career in research. Nguyen is deeply grateful for the unyielding guidance and support of Udayana Ranatunga and Dr. Nielsen, as well as Dr. Paul Pantano for his continuous mentoring.



## About the Contributors

## Tanushree Jhunjunwala

is a senior graduating with a bachelor's degree in economics in May 2012. She currently works as an undergraduate student researcher at the UT Dallas Center for Behavioral and Experimental Economic Science (CBEES). She became aware of her passion for research in her junior year when she started analyzing survey data for a project with Dr. Nathan Berg in which they attempted to predict academic success rates of students enrolled in economics courses. She found further motivation when she joined the CBEES lab and started working under Dr. Catherine Eckel on projects like "When is Inequality Fair?" and "Estimation of the Probability Weighting Function." Her professors have been a big source of inspiration to her. In her spare time, she likes to hang out with friends, dance, sketch, cook, and be anywhere close to nature. She loves traveling and intends to travel around the world. After her graduation, she plans to pursue a doctorate in economics.



# About the Contributors

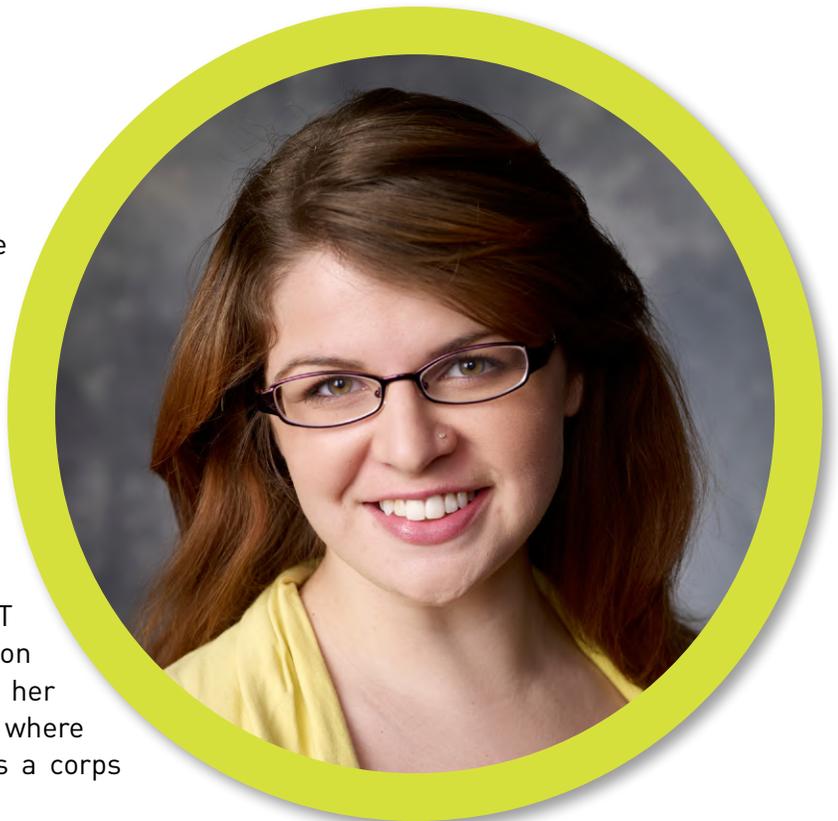


## Zachary Johnson

is a junior business administration and marketing major from Beeville, Texas. He is a proud Terry Scholar at UT Dallas. In his free time, he enjoys playing sports, reading, and swimming. Johnson plans on attending graduate school for his MBA soon after graduation.

## Brittany Sharkey Andrews

is a senior in art and performance. She holds minors in environmental studies and political science as well. Her interest in writing began when she was given a journal at age nine. By age eleven, three of her poems were selected for publication by various printing agencies. Since then, Sharkey has ventured her talents into research for the School of Arts and Humanities, performance poetry, and memo-writing as the current UT Dallas student government president. Upon graduation with school honors, she and her husband will move to Washington D.C., where she will be teaching special education as a corps member of Teach For America.



# About the Contributors

## Rebecca Aguilar

is a junior geosciences major. Born in Mexico and raised in the U.S., Aguilar is fluent in both English and Spanish. She enjoys reading, drawing, singing, and editing for the student publication *A Modest Proposal*. You will frequently find her in the office of *A Modest Proposal* sharing the company of an awesome drawing tablet and a geology book.



## Carrie Crossley

is a double major in arts and technology and computer science from Southlake, Texas. She was paired with Dr. Marjorie Zielke's lab through the UT Dallas Clark Summer Research Program, and she greatly enjoyed her time working on the First Person Cultural Trainer (FPCT). Crossley plans to continue studying arts and technology through graduate school, and hopes for a future in the field of game development. She would like to thank her family and friends for their constant support, as well as the FPCT team and Clark program directors for providing her with such an amazing opportunity.



# An Interactive Toolbox for the Analysis of Volcanoes on Earth and Mars

by Emily Butler

The use of three-dimensional (3D) digital information for analyzing geologic features on the surface of the Earth has been revolutionized over the past two decades with the advent of satellite-based observational platforms. As a necessary and natural extension, these technologies have been launched for planetary exploration, providing researchers with unprecedented access to spatial data.

This research seeks to further the analysis of volcanoes on Earth and Mars by creating an interactive software-based toolbox. The project is motivated by the fact that the volcanoes on Mars (which are inactive) provide a historical database that can improve our understanding of our own planet

Earth. Volcanoes on Earth and Mars have many similarities and differences, yet comparative data on these volcanoes are not easily accessible. There are separate databases of information on Martian volcanoes and volcanoes on Earth, but there is very little that combines the two. Also, information such as elevation and diameter of a volcano is rarely found in the same place as satellite images. The development of an interactive toolbox greatly facilitates our understanding of the historic and ongoing processes inherent on our own dynamic planet Earth. This will construct a platform to learn about the Earth and Mars as planets that may be more similar than meets the eye.

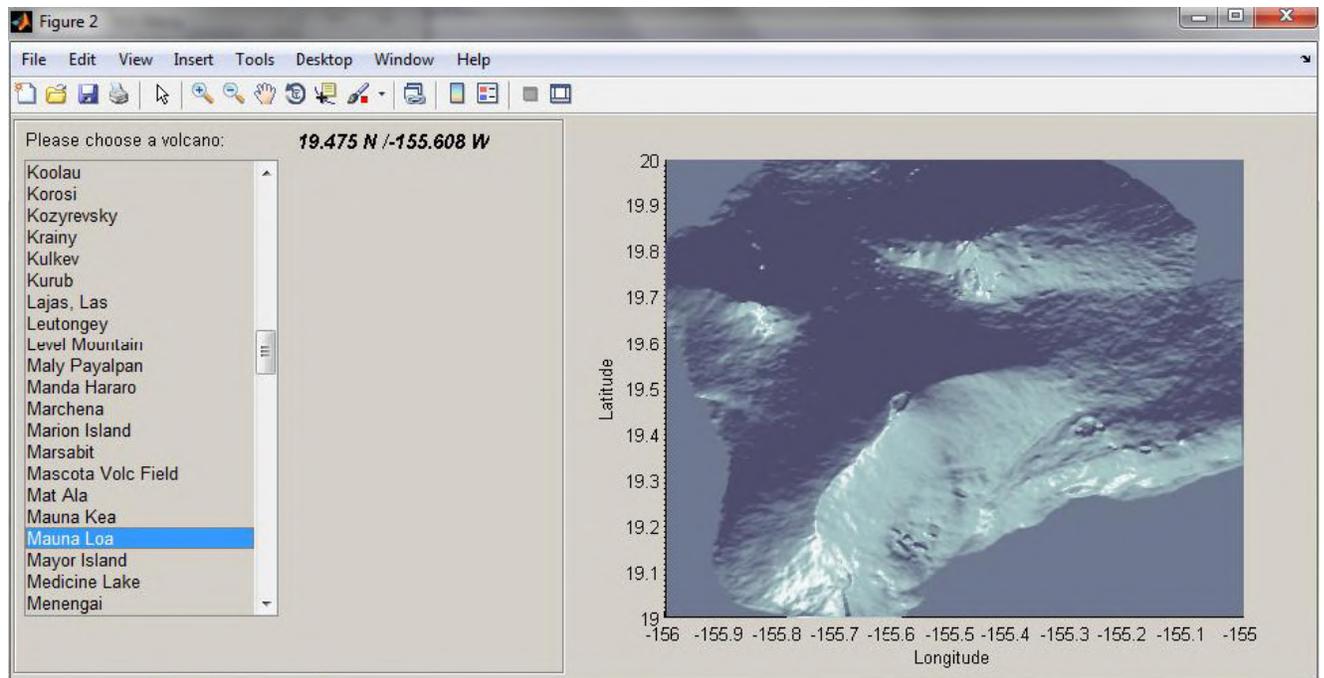


Figure 1. SRTM image of the Mauna Loa volcano

## Comparing the Earth and Mars

Earth and Mars have many similarities that make them ideal to compare for scientific purposes as opposed to using another planet in our solar system. The two planets have the same amount of land surface area despite Mars being a little over half the size of the Earth. They also have a similar atmospheric chemistry, sustained polar caps, historic evidence of climate changes, axial tilt (differing by a couple degrees), and seasons due to the tilt of the planet.<sup>1</sup> Because the two planets are so alike, they provide an easy comparison about an extensive range of topics, including volcanoes.

Discovering the physical features of volcanoes on the two planets allows for classification categories to include in the toolbox. Viewing two volcanoes in particular, one on Earth and one on Mars, gives the general idea for what differences to expect when comparing data from the two planets. For example, the most extensively studied volcano on Mars is Olympus Mons. It resembles a shield volcano and is the largest volcano on Mars, its peak reaching above the Martian atmosphere. From the surrounding plains, it is 23 kilometers in elevation.<sup>2</sup> The volcano on Earth most closely resembling Olympus Mons is Mauna Loa of the Hawaiian Islands. It is also a shield volcano but its elevation is only 10 kilometers from the base of the Pacific Ocean.<sup>3</sup> Despite the elevation difference, the two volcanoes are comparable in terms of their processes and physical features. Using these two volcanoes, the necessary volcano classification categories to be included in the toolbox are evident: the volcano's name, type, elevation, diameter of crater, latitude, longitude and location on the planet.

Identifying the coordinate system used for Mars was the next important step. Earth has an accepted geographic coordinate system while Mars has two approved coordinate systems: planetographic and planetocentric. Planetographic longitude, which is traditionally used, increases to the west and planetocentric longitude increases to the east.<sup>4</sup> Mars is also divided into quadrangles along latitudinal and longitudinal lines. Knowing the quadrangle where

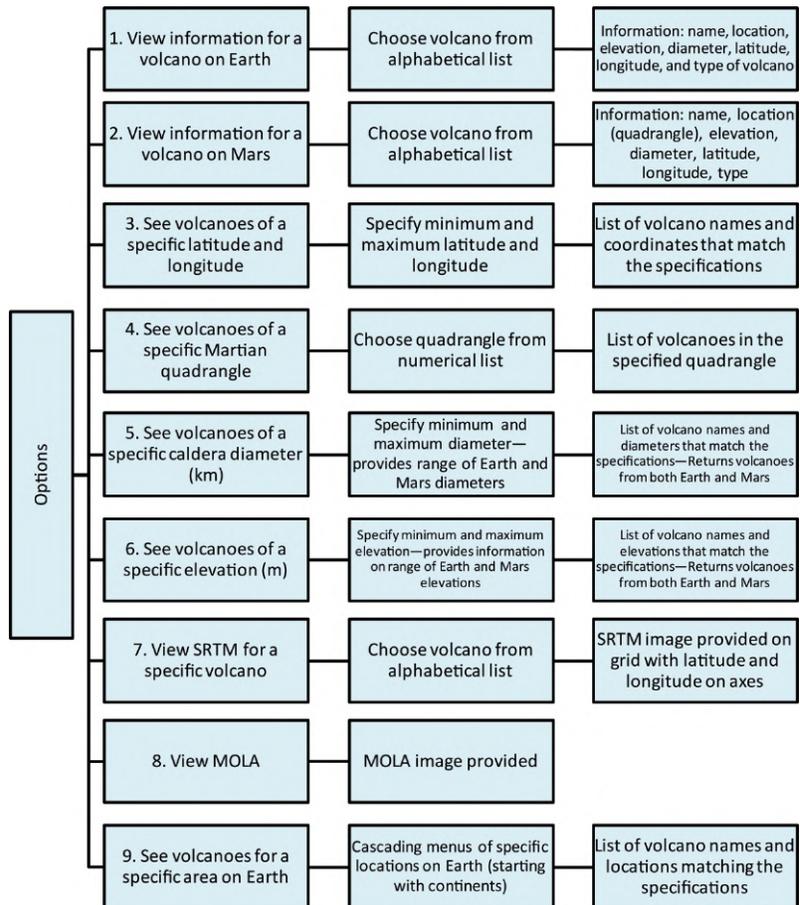


Figure 2. Flowchart of program options

a volcano is located can make it easier to refer to a volcano or volcanic field on Mars.

In order to compare volcanoes on Earth and Mars, one must understand the differences in volcanic processes. Earlier, Olympus Mons and Mauna Loa were compared. Olympus Mons dominates Mauna Loa in elevation and diameter. The reason for this is because Mars does not have plate tectonic motion. On Earth, and specifically in the Hawaiian Islands, theory says that the tectonic plate moves over the mantle's hot spots, creating a series of volcanoes in a line that correlates with their ages. New volcanoes develop as the mantle rises as plumes. In Mars' past, however, there is no driving force for plate tectonics.<sup>5</sup> This causes the mantle plumes to remain in the same place, resulting in a greater buildup for a volcano.<sup>6</sup>

## The Shuttle Radar Topography Mission and the Mars Orbiter Laser Altimeter Missions

Over 11 days starting February 11, 2000, the Shuttle Radar Topography Mission (SRTM) collected data and provided accurate information on a near global

basis. Using radar interferometry, SRTM data provided map information obtained in the form of a digital elevation model (DEM) of the Earth. The DEM from SRTM was at resolution levels of 1 and 3 arc seconds, or 90 meters over most of the world and 30 meters for the United States. The horizontal accuracy was 3 meters (better in most cases) and an absolute vertical accuracy, for a spatial scale of more than 500 kilometers, of about 10 meters. Both of these were much better than the expected error, which was 20 meters for horizontal measurements and 16 meters for absolute vertical. When creating the DEM, data from the STRM was averaged and mosaicked to further reduce error.<sup>7</sup>

From November 7, 1996 to June 30, 2001, the Mars Orbiter Laser Altimeter Missions (MOLA) collected high-resolution topography measurements of Mars. The MOLA instrument measured the time it takes for laser pulses to reach the Martian surface and be reflected back to the instrument. The resolution of this process was 37.5 centimeters on a smooth surface to about 10 meters on 30° slopes. The data have an absolute accuracy of 13 meters. With this accuracy, the global topography on Mars is known to greater accuracy than the continents on Earth.<sup>8</sup> Using this data, a 3D image of Mars was created, allowing the user to view the vast altitude variations on Mars.

### Development of Software Toolbox

The goal of this program is to facilitate the comparison of Earth and Mars through the use of volcano data. The interactive toolbox contains the most recent database of volcanoes and critical parameters (height, diameter, location and type, which includes shield and cone) on Earth and Mars and interacts with the user who will provide additional information to focus on specific volcanic ranges as well as interpretation. The volcanoes are visualized using digital terrain models of the Earth (obtained from SRTM) and of Mars (obtained from MOLA). Additional web-based resources such as Google Earth and Google Mars have been employed to verify and

expand the database. These databases and models are typically found using different resources and are usually separated by planet as well. By using the programming platform MATLAB, a suite of toolboxes was created in order to highlight these comparison points by bringing the database and imaging information together in a meaningful manner. This in turn allows for a wide variety of conclusions made by inferring conditions that existed on Mars and conditions that relate to Earth (i.e., hot spots and plate tectonics).

There are nine options in the toolbox that range from a database of volcano information to being able to view a volcano using SRTM and MOLA imaging (Figure 2). The first and second options in the toolbox provide a database of volcanoes on Earth and Mars, respectively. They provide an alpha-

*“The toolbox developed for this research will bring together modern technologies for data and create an environment in which to interpret them that has previously not been available. It will be used by researchers for advanced applications, but will also benefit educators who currently rely on sporadic resources that do not take advantage of advanced visualization techniques.”*

betical list of the shield volcanoes on Earth and all of the volcanoes on Mars. Only the shield volcanoes are included because they are the most similar to the volcanoes on Mars due to physical characteristics. After choosing a volcano from the list, the volcano's name, location, elevation,

diameter, latitude, longitude and type is shown. The third option allows the user to specify a minimum and maximum latitude and longitude, which will return a list of volcanoes and their coordinates that match the specifications. This only includes volcanoes on the Earth. In order to see volcanoes of a specific quadrangle on Mars, the user can choose a quadrangle from a drop-down menu in the fourth option. The fifth and sixth options let the user specify a minimum and maximum diameter and elevation, respectively, and returns volcanoes from both Earth and Mars that are within the intervals. The range of diameters and elevations is also displayed for volcanoes on Earth and on Mars. The seventh option provides an alphabetical list of volcanoes on Earth from which to choose and the SRTM image of the volcano chosen appears on a grid with latitude and longitude on the axes (Figure 1). The actual latitude and longitude is displayed for precise location. The eighth option shows the MOLA image of Mars,

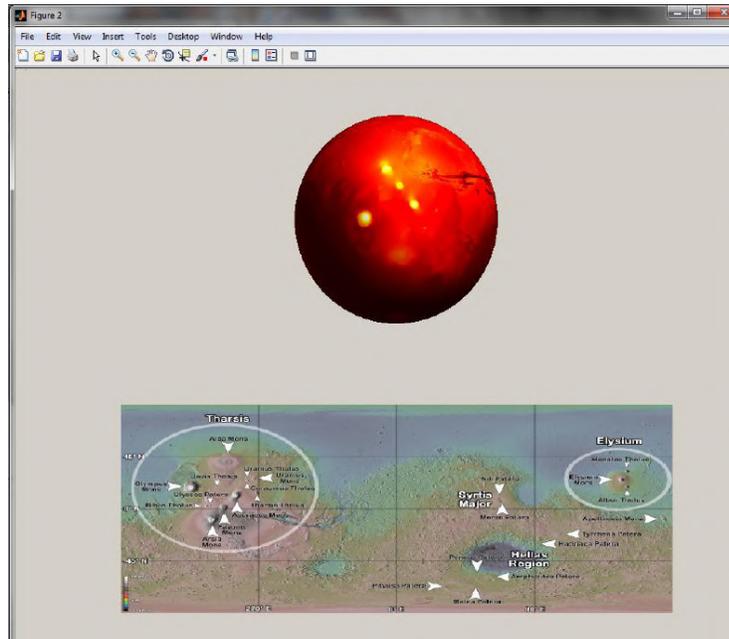


Figure 3. 3D rotatable MOLA image with reference diagram

which can be rotated to see the different quadrangles on Mars (Figure 3). The ninth option allows the user to specify a geographic location on the Earth (rather than latitude and longitude coordinates) and a list of volcanoes in that area of Earth will appear.

### Conclusions and Future Work

The toolbox developed for this research will bring together modern technologies for data and create an environment in which to interpret them that has previously not been available. It will be used by researchers for advanced applications, but will also benefit educators who currently rely on sporadic resources that do not take advantage of advanced visualization techniques. Logical deductions can be made through the use of the toolbox when applied to, for example, comparisons of elevation or digital models. It can be used for advanced applications that make use of the higher imaging processes or as a useful database of volcano information. Future work includes expanding the Earth volcano database to incorporate other types of volcanoes and allowing the user to add notes or take measurements from the imaging. The program will be published to MATLAB Central File Exchange and updated as new information is obtained.

### Acknowledgments

I would like to acknowledge Dr. Georgia Fotopoulos of the Department of Geosciences at UT Dallas for

hosting this research and providing valuable comments, as well as Martin Orlob for extensive help with the MATLAB programming platform.

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# Social Media Return on Investment: Tracking and Measurement

*by Zachary Johnson*

**W**ith over 800 million users on Facebook alone, social media have swept across the world in a wave of acceptance and seemingly limitless opportunity.<sup>1</sup> From the perspective of a firm or nonprofit organization, social media marketing (SMM) is a relatively inexpensive form of advertising performed on social media platforms such as Facebook, Twitter, LinkedIn, etc. Unfortunately, the problem with social media advertising is that managers have thus far only assumed its profitability without actual measurement of associated costs and revenues. The purpose of this research is to formulate a system to track and measure the return on investment (ROI) for SMM. This marketing includes but is not limited to contests, promotions, discounts, free samples, and advertising that occur on social media platforms.

Prior work by Trusov, Bucklin and Pauwels focuses on the elasticity of word-of-mouth (WOM) referrals, but does not isolate the social media variable in the calculation of revenue. Extraneous variables such as events and media appearances are included in the calculations, and as a result they “[cannot] make this distinction in [their] revenue calculations.”<sup>2</sup>

A WOM study performed with public data from the websites of Barnes and Noble and Amazon suggests that the difference in sales rank of a book across the two websites is related to the number of reviews and star ratings. The empirical evidence is limited in the sense that it “stops short of showing that retailers profit from providing such content.”<sup>3</sup>

Godes and Mayzlin note that there is a great amount of information that can be taken from com-

munication on the web. They develop an alternate method to measure online WOM using publicly available data on Usenet newsgroups and TV ratings from major broadcasting networks. The data are limited, but “in comparison to the social network mapping procedures, [their] data set offers an easy and affordable alternative.”<sup>4</sup> The social media mapping is a much more complicated and tedious form of measurement that has not been thoroughly explored.

Duboff and Wilkerson articulate the need for social media ROI tracking and measurement. However, they do not propose a method of actually tracking ROI. They merely assert that “everyone needs to monitor brand reputation in social media (and be ready to respond as needed), but not everyone should invest.”<sup>5</sup>

Throughout the studies, it is apparent that WOM affects the profitability of certain corporations. It is also noted that social media might affect profitability of corporations, but these presumed effects have not been quantified. In this paper, I will attempt to devise a method to measure the profitability of social media advertising. With my framework, firms and organizations would no longer invest their time and money in social media simply based on emotions or gut feelings; they would have specific, empirical data to guide their social media investment decisions.

## **The Deduction Method**

The total expenditures and returns of marketing may include but are not limited to print advertisements such as ads in magazines and newspapers;

broadcasting advertisements on radio and television; outdoor advertisements such as billboards and events; promotional advertisements such as new product promotions, coupons and related discounts; internet advertisements on various popular websites; and, lastly, SMM advertisements. To calculate the social media ROI, we need to net out returns on all non-SMM activities. On the costs side, ideally expenditures on social media marketing would be accounted for separately. However, in practice many firms and organizations do not keep track of SMM spending. The estimates of SMM expenditures and returns will likely be inaccurate since the costs and returns of other marketing activities may be measured incorrectly or their values may be unknown. These particular discrepancies may accumulate to form a large discrepancy between the estimated SMM expenditure and revenue figures and the actual figures.

ditures and returns, we will develop methods to directly measure the related returns on SMM ROI. We will also describe various ways to apportion SMM fixed and variable costs. With SMM expenditures properly estimated and a direct method of tracking and measuring returns, managers will be able to assess the profitability of SMM in comparison to other marketing strategies.



Figure 2. Stages of Social Media ROI. Image courtesy Effect Web Agency <http://www.effectwebagency.com>

Figure 2 shows stages of Social Media Return on Investment (ROI). A missing link exists between Investment and Implementation in the form of the need to calculate the expenditures that are required to implement a particular social media marketing strategy. Another missing link exists between Impact and Financial Gain in the form of the need to quantify sales revenue resulting from SMM. Taken together, these two missing links connect the real world of businesses and organizations to the social media world and provide marketers with a means to calculate return on investment.

The first step in estimating SMM expenditures would be to look at associated implementation expenses, salary expenses, as well as the costs of equipment, software and other related technologies. A firm or organization which is deciding whether to make the initial investment in SMM must first determine if it has the proper hardware and software. If not, it will need to purchase these necessities. After obtaining the proper equipment and software, the organization must dedicate a portion of a marketer's time to updating social media accounts. A portion of this marketer's salary will be taken into account in the calculation of SMM expenditures. Periodic expenses may occur with the need to replace du-

Total Returns from Marketing Efforts

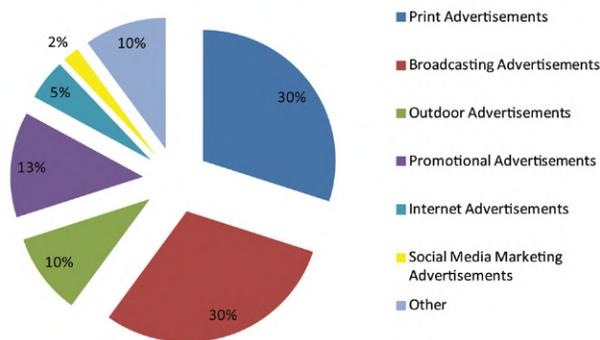


Figure 1. Example of deduction method

In the hypothetical marketing revenue pie graph shown in Figure 1, 98% of the total returns can be attributed to non-SMM advertising efforts. Through the process of deduction, 2% of the total returns can be attributed to SMM. This calculation may be inaccurate due to discrepancies in measurement or attribution of revenue to various marketing sources.

### Direct Measurement of Expenses

The direct method of tracking and measuring SMM ROI that we will develop will be more accurate than the deduction method, in that the accumulated discrepancies of non-SMM activities will not confound SMM measurements. Rather than netting out the SMM from the aggregate marketing mix of expen-

rable technology or to pay licensing fees associated with software.

In the second stage, the firm or organization should track all current, past and potential customer activity on social media platforms in response to social media marketing efforts. Examples of SMM efforts include marketer-generated comments, contests, promotions, customer impressions, word-of-mouth, reposting, etc. These SMM efforts are revenue drivers for the social media platform; therefore, they should ultimately result in increased sales. However, the link between online social media user activity and associated revenues (product sales) has not been established.

**Examples of Tracking for Direct Measurement of SMM ROI**

One simple method of tracking customers would be to post a uniform resource locator (URL) to an outside web page on a social media platform. The firm would track “clickstream data” from the point at which the customer leaves the social media platform to the point of purchase. This method offers firms a relatively quick and inexpensive way to track the customer’s activity and the direct correlation between SMM efforts and sales.

The second method would use web crawling programs, such as NetBase Insight Workbench, to directly collect information on WOM that users have posted on the Internet. These computer programs search social networking websites, online newsgroups, blogs and other social media, inputting every comment and response into a database. Using these databases, managers could analyze volume (number of comments) and dispersion (comments across different pages), as well as valence (positive or negative comments) and strength (strongly or weakly worded comments). They could then build a model that relates these WOM measures to sales.<sup>6</sup>

Another possible method would involve collecting profile information such as name, gender, age, location, etc. (to which customers grant marketers access when they “like” the firm or organization’s fan page) and matching the collected data with existing customer databases containing personal information and purchase history. The purpose would be to create a way for marketers to connect user comments to sales without a major strategic change in tracking, but any results would be of limited quality as many customers’ online and offline identities (or even online social media identities and online identities on other websites)

**Southwest Airlines**

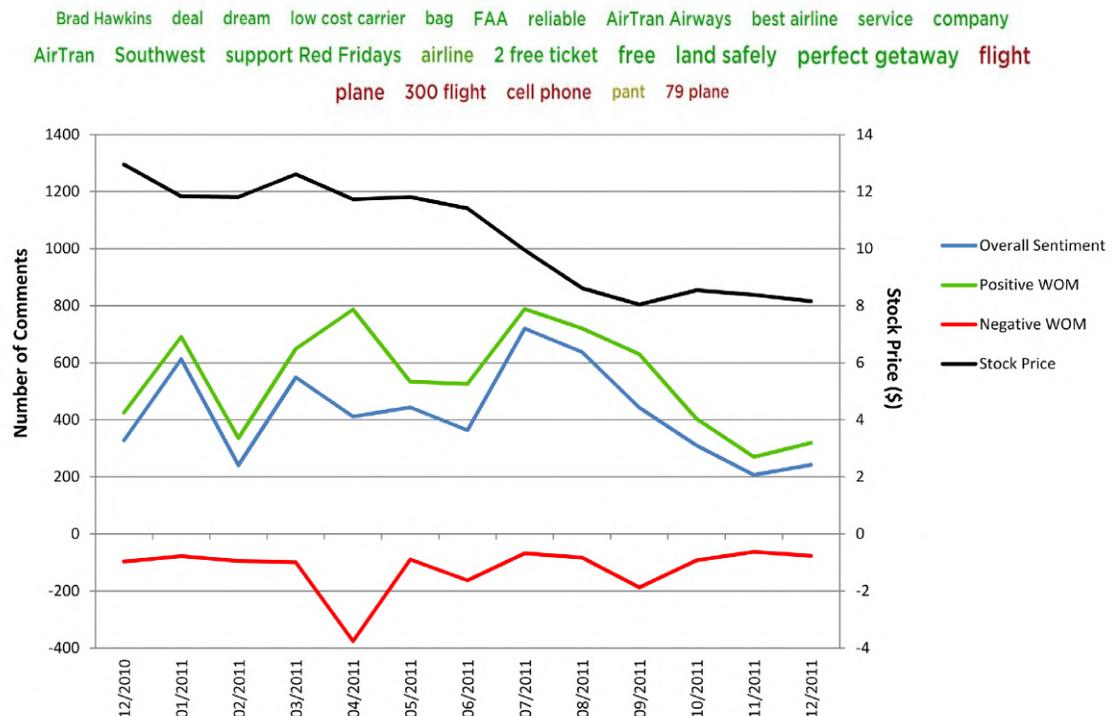


Figure 3. Overall sentiment and stock price for Southwest Airlines

would be extremely difficult to match. However, the method would provide a rough link between SMM efforts and existing customer purchases, despite the many non-matches. This method would be the most inaccurate form of direct measurement, but does not require the implementation of a new strategy to collect clickstream data off the social media platform.

**Analysis**

I am currently in the process of meeting with organizations to negotiate a partnership in social media ROI research. This collaboration will yield data on social media costs and revenues. In the meantime, I have proxied for these variables using annual advertising and revenue reported in 10-K filings. I have used NetBase Insight Workbench to measure the volume and valence of word-of-mouth across social networking sites, online forums, blogs, microblogs, news sites and other social media.

Figure 3 depicts positive and negative WOM, overall sentiment (difference in the number of positive and negative comments), and the monthly

average adjusted closing stock price for Southwest Airlines for a one-year period from December 2010 to December 2011. The “word cloud” above the graph is a visual representation of all WOM regarding Southwest Airlines. Green phrases in the word cloud represent social media users’ positive comments, yellow phrases represent neutral comments, and red phrases represent negative comments. The size of the phrase in the word cloud represents the number of times the phrase was used; the larger the word, the greater number of times it was mentioned by social media users. Southwest’s word cloud is primarily positive, with the exception of a few neutral and negative comments.

*“The problem with social media advertising is that managers have thus far only assumed its profitability without actual measurement of associated costs and revenues.”*

In measuring social media ROI, social media revenue is the missing link between Impact and Financial Gain, as previously discussed in Figure 2. As expected, Figure 3 shows that overall sentiment and stock price are positively correlated. Southwest’s 2010 10-K annual report notes that passenger revenues increased more than 16%, or \$1.6 billion, as a result of stronger management techniques and higher

**American Airlines**

FAA British Airways AAdvantage mile American free new company AA more service  
 save \$ 40,000 airline American Airlines flight suck American Airlines Flight 77 plane  
 American Airlines Flight 11 AMR American Airlines flight ticket lose luggage Alec Baldwin service offer  
 passenger

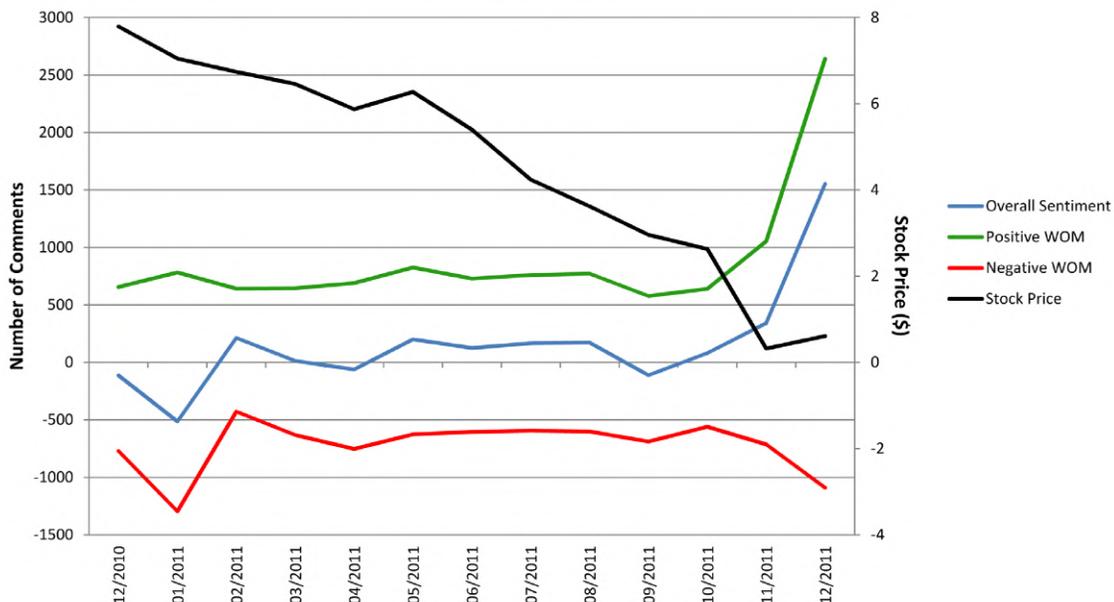


Figure 4. Overall sentiment and stock price for American Airlines

market demand for flights. SMM costs are the missing link between Investment and Implementation as previously described in Figure 2. Southwest's 10-K states that it decreased advertising expenditures by \$2 million from 2009 to 2010. It is possible that Southwest used social media effectively to maintain strong positive WOM and overall sentiments, even as the advertising budget was cut. Overall sentiment closely follows positive WOM, showing that positive WOM dominates negative WOM for Southwest Airlines.

Figure 4 shows the relationships among positive and negative WOM, overall sentiment, and the monthly average adjusted closing stock price for American Airlines for December 2010 to December 2011. American Airlines' word cloud is drastically different from Southwest Airlines', in that most of the comments about American Airlines are either negative or neutral. The adjusted closing stock price has a drastic downward slope for the entire year with a low of 32 cents in October 2011. Shortly after this yearly low, American Airlines filed for Chapter 11 bankruptcy protection on November 29, 2011. American Airlines' 2010 10-K reports an increase in passenger revenues of \$1.76 billion from 2009 to 2010. However, American Airlines' advertising costs increased \$12 million from 2009 to 2010, and the number of negative comments remained high in volume. This indicates the possibility that American Airlines is running an ineffective social media advertising campaign, in the sense that more money is being spent on advertising with little gain in overall sentiment. In contrast to Southwest Airlines, American Airlines' overall sentiment closely follows negative WOM (rather than positive WOM) from December 2010 until October 2011. American Airlines' monthly overall sentiments also hover around zero, which shows that customers feel either indifferent or negative toward American Airlines. The number of negative WOM comments was high in both December 2010 and December 2011; this may be due to high congestion and poor service during holiday travel or the recent bankruptcy announcement. It is interesting to note the drastic increase in both positive and negative WOM volume in December 2011, much of which is related to actor Alec Baldwin being escorted off an American Airlines flight for his refusal to turn off his cell phone. This shows that events beyond marketers' control can strongly affect WOM.

## Conclusion

There is a pressing need for firms to properly collect social media marketing data and track their marginal revenue from SMM efforts. This information is required for firms to calculate the profitability of social media marketing. With this information, the firms will be able to assess the success of their social media marketing and determine whether to reduce SMM effort and allocate money to other more profitable marketing strategies. Without this information, firms and organizations are essentially "flying blind" in that they believe that SMM efforts result in increased revenue but are unable to calibrate their efforts optimally.

## Acknowledgments

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# Antimicrobial Activity of Plant Extracts: How Common Vegetables and Oils Can Change the Way Diseases Are Treated

by Syed Muhammed Rasheed

Nature has been a potent agent for curing many diseases for thousands of years, and it has also been a topic of research in the pharmaceutical industry. This plant-based medicine approach plays a critical role in today's healthcare due to the many chronic diseases that affect people. When tissues in the body are injured a set of reactions immediately begins to repair the injured tissue in multiple ways. Inflammation is the natural biological response to harmful stimuli, such as pathogens. When a certain part of the body is injured special cells are recruited to release chemicals and other factors that help to remove the cause of the injury and repair the tissue. If this response becomes maladaptive, it can lead to progressive tissue injury such as fibrosis and organ failure.<sup>1</sup>

There are many anti-inflammatory drugs that work to reduce inflammation by suppressing the immune system. Unfortunately, this suppression may actually promote microbial infections. Antibiotics can be used to kill the pathogens; however, one of the downsides to using antibiotics to fight infections is that they kill not only the unwanted bacteria but also the "good" bacteria in the body.<sup>2</sup> This in turn causes other infections to develop in the body. For example, women are prone to yeast infections due to antibiotic use. Any woman may be at risk for a yeast infection if she takes an antibiotic for more than four or five days.<sup>3</sup> An additional downside

to using certain antibiotics is that sometimes the bacteria become resistant to the antibiotics.<sup>4</sup> As a result, the body never fully heals from the infection because the bacteria are still living in the body. This in turn can make the body more vulnerable to other infections and diseases.

Thus, the best way to reduce inflammations may be by using natural plant products, which can be anti-inflammatory without being immunosuppressive and can have the ability to fight certain pathogens by acting as effective antimicrobial agents. In this experiment, we examined the efficacy of using different groups of plant products to fight certain bacteria. We also investigated how the different plant products fared against each other and how they compared when they were used in combination.

Our aim was to find natural anti-inflammatory agents that also showed potent antimicrobial activity. An antimicrobial agent

is a substance that kills, prevents or even slows the growth of a microorganism.<sup>5</sup> Though there is much literature on the antimicrobial activity of many plant products, not much is known about how they compare and about their effectiveness when used in combination. For example, not much is known about how effective garlic and eucalyptus oil can be against certain bacteria when they are used in combination. Furthermore, not much is known about eucalyptus oil and its potential antimicrobial

*"The best way to reduce inflammations may be by using natural plant products, which can be anti-inflammatory without being immunosuppressive and can have the ability to fight certain pathogens by acting as effective antimicrobial agents."*

Chemicals	<i>S. aureus</i>	<i>S. pyogenes</i>	<i>E. coli</i>	<i>P. aerogina</i>
Tetracycline (Te 30 ug)	35 (mm)	No Growth	33 (mm)	10 (mm)
Trimethoprim (Tr, Tmp 5 ug)	25 (mm)	No Growth	33 (mm)	0.1 (mm)
Penicillin (Pe, P10 ug)	36 (mm)	No Growth	9 (mm)	0.1 (mm)
H2O (Water)	0	0	0	0
Eucalyptus oil (EU)	32 (mm)	40 (mm)	35 (mm)	11.5 (mm)
Garlic (GA)	35 (mm)	20 (mm)	25 (mm)	7 (mm)
Onion (On)	0	13 (mm)	0	0
Strawberries (ST)	10 (mm)	0	0	0

Table 1. Zones of inhibition for the chosen antibiotics and plant extracts against the chosen bacteria. All the plant extracts shown on this graph showed a zone of inhibition indicating antimicrobial activity. Note: mint, turmeric, ginger and tomato are not shown on the graph because they did not demonstrate a zone of inhibition.

effects against certain bacteria that we tested such as Salmonella typhimurium and Bacillus cereus. The identification of plant products with both anti-inflammatory and antimicrobial properties could have great potential to fight disease without the risk of infection.

**Materials, Methods and Designs**

The different plant products or extracts used for this experiment were mint, strawberries, tomato, turmeric, ginger, eucalyptus oil and garlic. These were chosen as they have been shown to have certain chemical compounds that are known to have anti-inflammatory properties. The bacteria tested against the plant products were Salmonella typhimurium, Pseudomonas aeruginosa and Escherichia coli,

which are Gram negative bacteria, and Staphylococcus aureus, Bacillus cereus, and Streptococcus pyogenes, which are Gram positive. The difference between the two types is that Gram-positive bacteria have thicker cell walls than Gram-negative bacteria.<sup>6</sup> This allows Gram-positive bacteria to retain a dye so scientists can differentiate them from other bacteria. The positive control antibiotics used in this experiment were Tetracycline, Trimethoprim, and Penicillin, and the negative control was water. All the plant products that were used in this experiment were organic.

Controls are important in any experiment because they allow us to measure the effectiveness of our treatment. All methods and preparations used in this experiment followed accepted testing

Chemicals	<i>S. aureus</i>	<i>S. pyogenes</i>	<i>E. coli</i>	<i>P. aerogina</i>
Eucalyptus oil (EU) & Garlic	33.5 (mm)	30 (mm)	30 (mm)	9.25 (mm)

Table 2. Zone of inhibition averages of Garlic and Eucalyptus oil when used in combination. Note: Combination of Garlic and Eucalyptus oil displayed the greatest zone of inhibition average against *S. aureus*.

standards, and some parts of the experiment were repeated to ensure that the results were accurate and precise.

### Plant Collection and Extract Preparation

All the plant products were extracted by crushing the plant using a mortar and pestle to squeeze out the juices. The mint juice was extracted a little differently – by pulling off the leaves of the plant first and then pulse blending them – because we did not want to have any damage to the extract due to a rise in temperature, as heat could denature the active substances in mint. Equal amounts of each of the plant extracts were collected. After the extracts were collected in individual test tubes, they were stored overnight at 4°C in the refrigerator. Test tubes were used to store our different plant extracts. Small filter disks were then placed in each extract a day before the experiment and put back into the refrigerator at 4°C for 24 hours. Putting the filter disks in the test tubes that contained our different plant extracts for 24 hours allowed the disks to absorb the plant extract juices. This in turn caused the disks to become saturated.

### Experimental Design

Mueller Hilton plates were used for our experiments and were divided into four groups. Each plate in the group was labeled with the names of each of the four bacteria (*E. coli*, *S. aureus*, *S. pyogenes* and *P. aeruginosa*), and all the plates were divided into four equal quadrants. The filter disks that were soaked in the different plant extracts were then placed in each quadrant. We also divided the four control plates into four cross-sections for positive control antibiotics and negative control water. The next day the bacteria were spread through the plates with a cotton swab. To avoid any contamination, we used different swabs each time we spread the different bacteria on the plates. Next, the soaked disks were placed in the middle of the plate. Then the plates were placed in a 30°C incubator for two days to see if any of the natural plant products could kill/stop the growth of bacteria. The decision to incubate the plates at 30°C for two days rather than 37°C was to reduce the chances of an overgrowth whereby the opportunistic pathogen's growth would negate any

type of antimicrobial properties. The results were obtained by measuring the zone of inhibition (in millimeters) and comparing it to the zone of inhibition exhibited by the positive control antibiotics. The zone of inhibition is an area on an agar plate where growth of an organism is prevented or slowed by an antibiotic placed on the agar surface.

The second part of the experiment involved the setup of serial dilutions of plant extracts that showed the most antimicrobial activity in the first part of the experiment: garlic and eucalyptus oil. The same procedure was repeated for this part of the experiment except that two additional bacteria (*B. cereus* and *S. typhimurium*) were added to the experiment. Serial dilutions were made from the

original stock of garlic and eucalyptus oil extracts, which was around 9 mL. In this part of the experiment, we performed a 1 in 10 dilution. After the dilutions

were made, the same procedures were followed as described above for the first experiment. The agar plates were divided into four cross-sections and labeled left to right from the most concentrated to the least concentrated plant extracts. The zones of inhibition were measured again to confirm our results and to see if the zones of inhibition were affected by increasing the concentration of the plant extracts.

### Results

From Table 1 it can be seen that out of all the plant extracts tested, garlic and eucalyptus oil demonstrated the most potent antimicrobial activity. The antimicrobial activity of these extracts was seen in all the bacteria with garlic exhibiting maximum effect on *S. aureus* and *E. coli* with an average of 31.6 and 19.6 mm zones of inhibition while eucalyptus oil had an average of 32.8 and 34.1 mm zones of inhibition. Eucalyptus oil showed larger zones of inhibition with *E. coli* and *P. aeruginosa* than garlic, and the organism most affected by both garlic and eucalyptus oil was *S. aureus* (Table 1). Thus, we found that eucalyptus oil and garlic work best when used in combination with each other against certain bacteria (Table 2). Garlic and eucalyptus oil achieved the greatest zone of inhibition when their zone of inhibitions were averaged together. One of the most fascinating findings from our experiment

*“Some of the plant extracts demonstrated larger zones of inhibition than some of the antibiotics.”*

was that some of the plant extracts demonstrated larger zones of inhibitions than some of the antibiotics. For example, Table 1 shows that eucalyptus oil had a larger zone of inhibition than Tetracycline. To confirm our results from the first part of the experiment we also performed a dilution test and also added two more organisms, *S. typhimurium* and *B. cereus*. The results were similar and supported our findings. Furthermore, the dilution test gave proof of the effectiveness of garlic and eucalyptus oil. The results clearly showed that the zones of inhibition decreased with decreasing concentrations of the plant extract. Thus, we found out that garlic and eucalyptus oil are most effective at killing bacteria when they have the highest concentration of plant extracts.

### Conclusion and Implications in Medicine

The experiment described in this article provides evidence of the potent antimicrobial activity of garlic and eucalyptus oil. Allicin is the main active compound found in garlic. It has been shown to be useful for treating skin infections.<sup>7</sup> Eucalyptus oil

has been shown to have antiseptic properties and has been used to treat ear infections.<sup>8</sup> This type of experiment is important in the field of biology and medicine because it can help scientists and physicians find cures to certain diseases. With these kinds of experiments we can find out which plant products are the best at killing certain bacteria. The identification of plant products with both anti-inflammatory and antimicrobial properties could have great potential to fight disease without the risk of infection. As for the future of this research, scientists can further their understanding by using combinations of extracts and also begin testing on human cells. According to the World Health Organization, medicinal plants would be the best source to obtain a variety of drugs.<sup>9</sup> Therefore, it is critical that more experiments like this are carried out by scientists to better understand the properties of plants in curing a variety of diseases. With these positive results we can move on to other experiments to better understand the antimicrobial properties of plants.

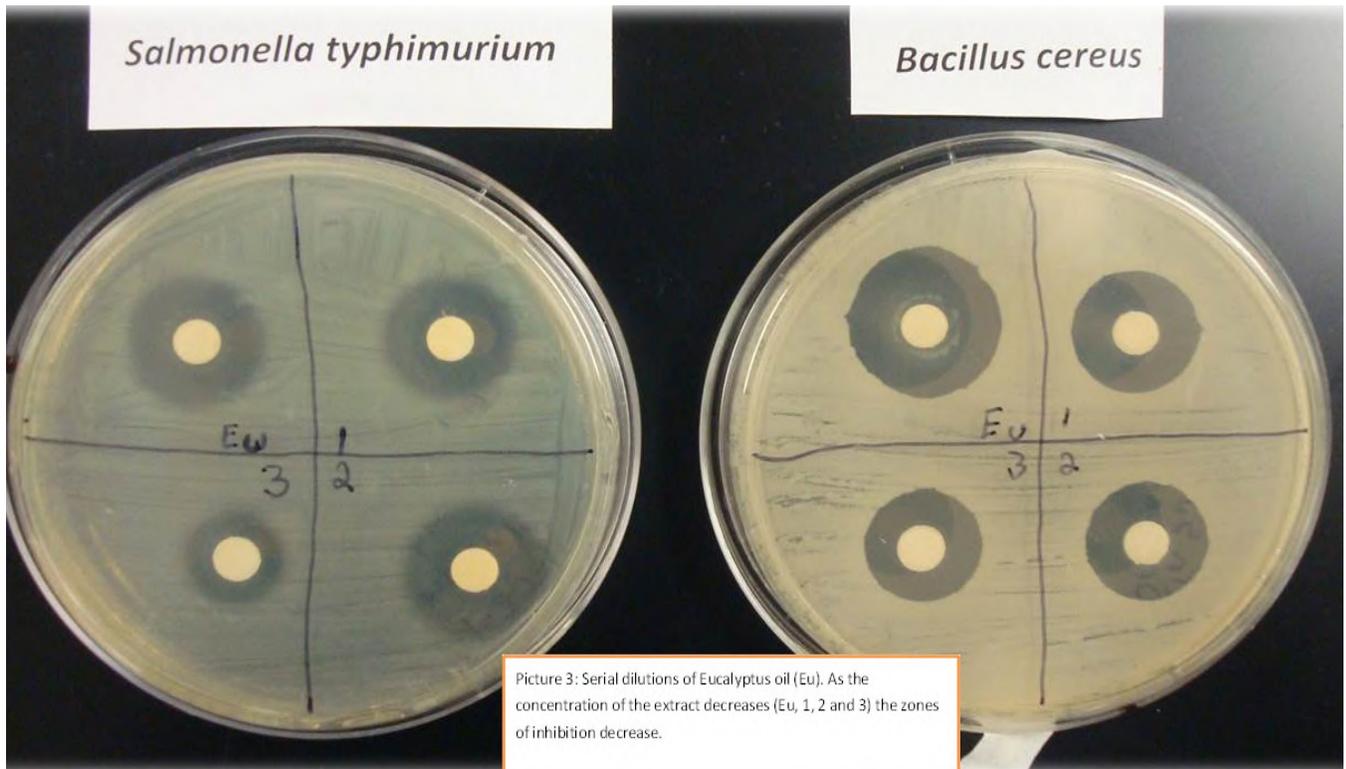


Figure 1. Serial dilutions of Eucalyptus oil (Eu). As the concentration of the extract decreases (Eu, 1, 2, and 3) the zones of inhibition decreases.

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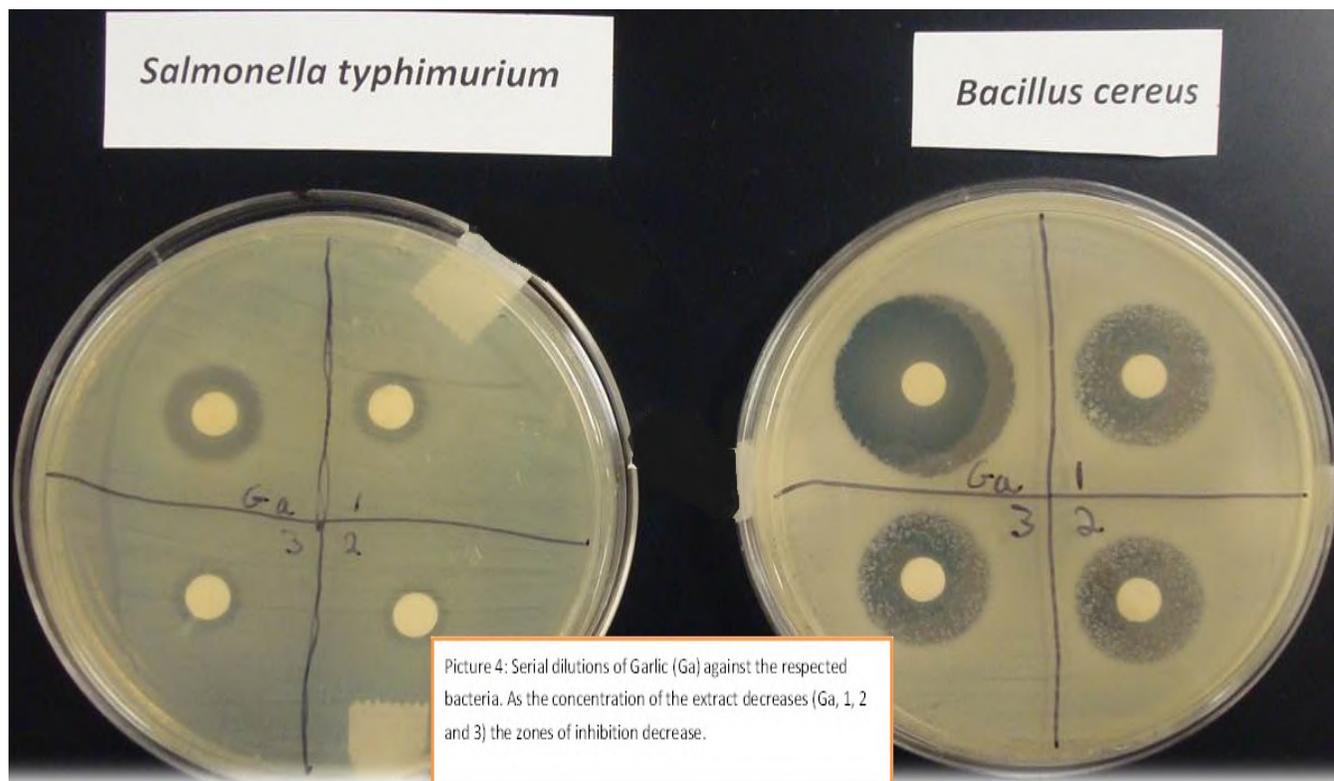


Figure 2. Serial dilutions of Garlic (Ga) against the two bacteria. As the concentration of the extract decreases (GA, 1, 2, and 3) the zones of inhibition decrease.

# I'm In Ur Jurnuhl, Anuhlizing Ur LOLcats: LOLcats Fandom and American Culture

by Larissa Weidenbruch

**A** plump, fluffy gray cat stares at you inquisitively. "I can has cheezburger?"<sup>1</sup> he asks. This is the first LOLcat, born on January 11, 2007, and it revolutionized the way we look at cats. A LOLcat is an image of a cat with a witty caption depicting the thoughts of the cat in that scenario. I argue that through its new language variety and its rapidly evolving, self-reflexive fan text, the LOLcat meme represents a new kind of fan object and an expansion of the participatory function of fan culture. LOLcats fulfill personal, cultural and social needs for fans including identity formation, commemoration of classical cultural production and a social community. Most importantly, these functions provide a utopian space for fans as a contrast to their offline lives.

Ben Huh, The CEO of Cheezburger Network, the site that hosts LOLcats, describes LOLcats as "Garfield, but as reality television."<sup>2</sup> You will know a LOLcat when you see one because it includes an

intriguing picture of a cat with a witty caption typed in the font "Impact or Arial Black,"<sup>3</sup> usually in white or black. This simple, straightforward appearance gives the captions the impact of one-line zingers or concise puns. This caption is written in a language called "lolspeak,"<sup>4</sup> which uses "deliberately bad grammar"<sup>5</sup> stemming from "a mixture of texting,

Internet hacker language, and just misspellings"<sup>6</sup> to capture the "imaginings of cats' inner monologues."<sup>7</sup>

LOLspeak is linguistically significant because it is not merely misspelled words and illiterate babblings, but a language variety that contains graphic, orthographic, grammatical, lexical, and discourse features.<sup>8</sup> The term "LOLcat" is itself a linguistic amalgamation. The word is formed by compounding the

two free morphemes "LOL" and "cat," where the term "LOL" is an acronym for "laugh out loud" and is used to indicate something funny or ironic, in this case modifying cats.

Furthermore, LOLspeak has a fairly regular

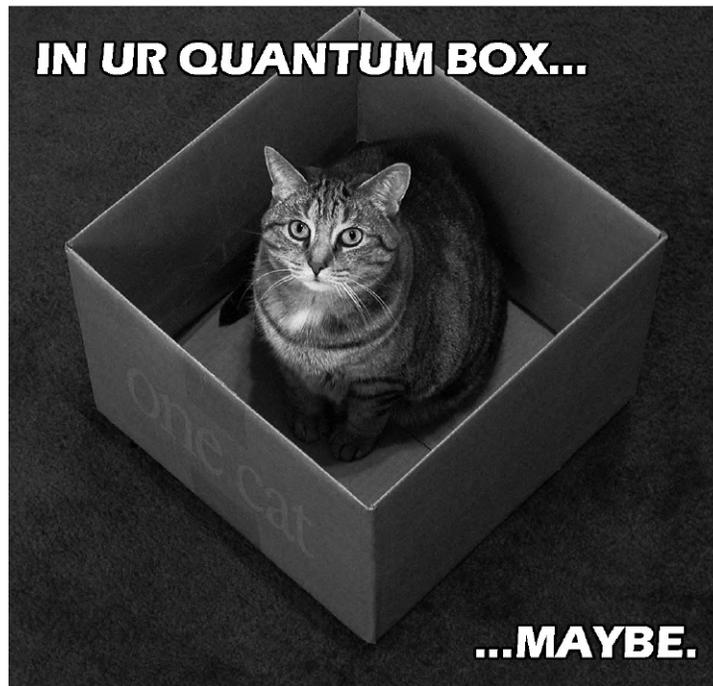


Figure 1. A box for every cat.  
© Photo Kevin Steele. Caption Dan Lurie.

system of spelling and includes purposeful common typos, such as “teh” for “the” and “pwn” for “own,” which allude to the fast-paced world of the Internet. LOLcats feature the phonetic spelling of words by using many double letters, changing “s” to “z,” and including superfluous vowels, all of which fill in the prosody missing in keyboard restricted conversations. Exclamation points and repeated letters add emphasis, slow the pace of reading, and can convey a tone of frustration, excitement or uncertainty. In addition to spelling errors, LOLcats have intentionally and consistently incorrect verb conjugation.

LOLcats also have lexical features, a “set of words and idioms given distinctive use within a variety”<sup>9</sup> to convey meaning, including shortened forms of words, misuse of homonyms, and dropped articles.

The use of this language variety differentiates LOLcats from other image macros—“an image with varying text.”<sup>10</sup> An image macro is a type of meme, “a unit of cultural transmission, or a unit of imitation.”<sup>11</sup> A meme on the Internet can take almost any form, from a “phrasal template,”<sup>12</sup> like a snowclone, an image macro, a video, or any other “viral online phenomenon[on]” as long as it conveys “bits of cultural shorthand.”<sup>13</sup>

LOLspeak and the viral meme combine in LOLcats to attract many fans. Henry Jenkins describes fandom as hunting an interest within a text and shaping it into an original creation, an act he calls “poaching.”<sup>14</sup> This synthesis places fans as active consumers of the fan object, such as a movie, book, or TV series, and validates their work. However, LOLcats deviate from traditional fan objects in their self-reflexivity and their rapidly evolving content.

LOLcats, unlike television series or films, do not have a consistent text; instead, they are amalgamations of image macros created by fans. LOLcats are a kind of poaching from popular culture because most images are inspired by other memes, advertisements, songs or TV shows. Fans create entire storylines that thread the image macros together into their own fan text and build on others’ stories in the comments thread. Then, contributing to the rapid evolution and self-reflexive nature of LOLcats,

*“The distance created by using the proxy of cats is the essence of this utopian society that LOLcat users have built around this meme because it provides a buffer that allows users to comment on pertinent and controversial issues without the threat of typical repercussions.”*

fans poach that content to create new memes, build their own LOLcats, translate famous texts into LOLspeak like the LOLcat Bible, etc. The process that drives this reflexivity within LOLcats is similar to Jenkins’ analysis of a politically charged Photoshop image that circulated the Internet, which took on “unpredictable and contradictory meanings” that accompanied the “decontextualized and recon-

textualized” text and images “at the sites of consumption.”<sup>15</sup> This reflexivity and deviation from a typical fan object allow for more participation because fans create the fan object and then respond to these objects by creating fan texts in response.

Because of this increased participatory role and the language variety, I argue that LOLcats serve personal functions, cultural functions and social functions for fans. One example of a personal function of LOLcats is providing a forum for identity formation. Baym argues that identity formation is a positive trait of online communities because “it creates opportunities to invent alternative versions of one’s self and to engage in untried forms of interaction.”<sup>16</sup> LOLcat fans can select a username and photo that give insight into the features or nicknames that a fan uses as self-identification. Also, users can create a profile page similar to other social networking sites with a news feed of the current activity including posts, comments and pictures that the user liked. On the profile page, there is a sidebar that includes an “about me” section, trophies, collectibles, statistics, friends and messages. The trophies are awarded for different milestones of membership including “I Made a Funny,” earned by submitting an image macro, and “Belle of the Ball” to mark different numbers of friends acquired. The statistics detail how many people have added a user as a favorite and how many different images the user has uploaded. The collectibles are images that a user can collect or give as gifts.

Taken together, these parts of the profile build an identity for the fan. An online identity “may have little correlation to the identity of the person”; however, this allows fans the freedom to “present themselves strategically” and have more control

over how they are perceived by others.<sup>17</sup> Although this seems deceptive, people present themselves in a certain way in different face-to-face social situations “in order to accomplish their short-term and long-term goals.”<sup>18</sup> One way LOLcat fans personalize their pages and define their identities is by choosing which collectibles to keep, thereby defining what they deem important and showcasing this for other members to see. The LOLs (the term given to any image macro from the host site Icanhascheezburger.com) that the user likes show up on the profile news feed, providing a mosaic of images that, when pieced together, form a sense of the individual and his or her personal preferences. The ability to create an identity online allows users to sidestep the ever-present “interpersonal identification and judgment process by which we normally evaluate each other in face-to-face interaction” and the subsequent “mistrust brought on by visual markers of difference.”<sup>19</sup> For LOLcat users, this ability to control and determine how a public views individuals is a factor contributing to the democratic ideals underlying this community that attempts to create a utopia not present in users’ everyday lives.

Parallel to this formation of identity, LOLcats serve the cultural function of commemorating classical cultural production by recreating them with cats. These allusions are sometimes difficult to catch if the viewer is unfamiliar with the work. This process reveals the relatively high intelligence of LOLcat users to craft such artful allusions and puns, despite the fact that they communicate in a language that appears to be butchered English. Jenkins remarks that creating “critiques or spoofs” provides a medium that “offers more localized channels for responding to that culture.”<sup>20</sup> Recontextualizing classical cultural production within LOLcats allows users this medium of response that Jenkins mentions by providing a safe distance attained through the proxy of a cat picture to discuss potentially controversial topics.

For example, Figure 1 features a cat in a box with the caption “In ur quantum box...Maybe,”<sup>21</sup> alluding to the Schrödinger’s Cat thought experiment. To the educated eye, this image juxtaposed

with the caption immediately produces a humorous interpretation; however, one must be able to recognize the significance of a cat in a box paired with the uncertainty of its existence. The thought experiment attempts to explain the paradox of quantum mechanics where electrons “enact simultaneously all the possibilities predicted by the equation, thus existing in a superposition of states.”<sup>22</sup> Comparing this idea to a cat in a sealed box with a vial of poison, an observer must assume that the cat is both alive and dead because of the uncertainty of the situation. This LOLcat displays a deep cultural literacy as well as creativity to reinvent a work and set it in a new context.

Furthermore, some LOLcats comment on the political process. The fact that people turn to this form of communication to express political ideas may indicate that some people feel more effective acting through an Internet meme than through the democratic system. This supports the

*“Contrary to these fears that the Internet and memes like LOLcats spark the downfall of intelligence, this meme serves to reinforce cultural literacy and show a strong command over the content.”*

idea that LOLcat fans are participating in a type of utopia that is separate from their traditional interactions with society. Jenkins emphasizes this idea of “digital democracy” through “hybrid spaces” with his discussion of the appeal of Photoshopped images as political statements, “where we can lower the political stakes (and change the language of politics) enough so that we can master skills we need to be participants in the democratic process.”<sup>23</sup> LOLcat fans perform a similar process of embracing democratic processes and spreading a political message through the hybrid space of image macros by relating the political jargon to the context of what they understand and the meme itself. Despite fans embracing the democratic concepts of voting for posts and voicing opinions within the LOLcats community, there is a schism when it comes to the politics of the world outside of LOLcats because some LOLcats fans believe this process infringes on their utopian space.

This genre of LOLcats refutes the comments left by some critics of LOLcats:

“As the extinction process marches merrily on leaving nothing living in its wake, so goes the human mind. Understand that I like ICHC [I Can Has

Cheezburger], but it is just another testament to the dumbing down of humanity...<sup>24</sup>

Contrary to these fears that the Internet and memes like LOLcats spark the downfall of intelligence, this meme serves to reinforce cultural literacy and show a strong command over the content. At the same time, they also create a utopian environment where this type of knowledge and creativity is respected, appreciated and applauded.

Encompassing and underlying these functions is the opportunity to share this experience with others. The social community of LOLcats allows members to support each other, commiserate with critical self-analysis, reinforce cultural critique, praise cultural production, and share creative products. There is much debate in the scholarship about whether online interactions constitute communities because of the facet of one definition of community that incorporates a proximal space. However, Fernback argues that “cyberspace has dimensionality, continuity, curvature, density, and limits” so that “virtual space is socially constructed and re-constructed space,” giving room within the definition for online interactions.<sup>25</sup>

Baym defines a virtual community as one in which users “exploit the systems’ features so as to play with new form[s] of expressive communication, to explore possible public identities, to create otherwise unlikely relationships, and to create behavioral norms.”<sup>26</sup> Members of the LOLcat community communicate through LOLspeak, build their profiles to explore public identities, bond with members from all over the world, and create behavioral norms like the role of the asterisk to imply action in comments, the terminology for making new friends by saying “\*extends floofy paw of friendchips\*,”<sup>27</sup> and the supportive atmosphere of the LOLcat community. Strangelove, in his analysis of YouTube fandom, also points out the role of “storytelling” as creating “its own self-referential, reflexive culture.”<sup>28</sup> Within LOLcats, this reflexive nature of storytelling further binds the community together because it creates layers of in-jokes that only fans who have been there through the multiple evolutions can grasp, thus encompassing the idea of collective intelligence that Lévy stresses as integral to community formation.<sup>29</sup> Members follow a behavioral protocol and support each other as in traditional communities, whether on or offline.

But why do we care that so many people find

personal, social, and cultural satisfaction from this meme? Far more than Huh’s stated purpose “to make people happy for five minutes a day,”<sup>30</sup> LOLcats are significant beyond the scope of a pastime at work or inspiration for a project because they create a utopian space as a supplement to real life, provide connections in a technological world, and demonstrate cultural literacy. Jenkins identifies fans as “overeducated for their jobs” and “not challenged by their professional lives,”<sup>31</sup> which applies to many LOLcat users who frequent their created utopia to seek this type of intelligent indulgence. LOLcats allow viewers the opportunity to escape their real lives to make a critical statement, question the intention of a work, extend the artist’s vision, create an alternative interpretation, and play with the original idea within the safe haven of a LOLcats thread. Jenkins identifies the “critique of conventional forms of consumer culture”<sup>32</sup> as the purpose of fandom, and he argues that parody allows fans to “bring the issues down to a human scale,”<sup>33</sup> which is the same process that the recontextualization of a classical cultural product into a LOLcat serves. The distance created by using the proxy of cats is the essence of this utopian society that LOLcat users have built around this meme because it provides a buffer that allows users to comment on pertinent and controversial issues without the threat of typical repercussions.

In addition to this utopia, which supplements the deficits present in modern life, LOLcat fans find connection, communion and support in this increasingly mediated existence. This safe audience of like peers and the participatory nature of LOLcats empower fans to participate in a rewriting process that displays a sense of cultural literacy. Jenkins argues that fans have the ability “to meaningfully impact the flow of ideas”<sup>34</sup> by changing “commercial culture” by “writing over it, modding it, amending it, expanding it, adding greater diversity of perspective, and then recirculating it, feeding it back into the mainstream media.”<sup>35</sup> This is the process apparent within the recontextualization that LOLcat fans use to reinvent classical cultural production. Far from corrupting these forms, this process serves to preserve and resituate the idea in a more modern context. This opens up the idea for discussion as to its current role in society and propels the viewer to consider the fluid nature of knowledge that they had previously held fixed.

## Acknowledgments

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# Solar Powered Water Purification System

by Matthew McCann

**A**pproximately 900 million people live without safe drinking water.<sup>1</sup> This truth is sad, yet it is a solvable problem. Rural areas lack access to stable power and water supplies. Therefore, a viable solution must harness energy from the environment and use it to purify water. The final product must also be rugged, inexpensive and easy to use.

The idea for this project arose from the 2011 International Future Energy Challenge which called for a “low power induction motor drive system supplied from a single photovoltaic panel for an emergency water treatment device.”<sup>2</sup> The first versions of this project were designed and built by a consortium of students from UT Dallas and Texas Christian University (TCU). The final product produced by that group reacted to changing light profiles and had over 90% efficiency. The design is now being modified at UT Dallas to attain even higher efficiency and fit other uses.

The objective is to build a power electronics converter (labeled “Converter” in Figure 1) that will take power from the photovoltaic panel and process it to drive an induction motor.<sup>3</sup> That motor will turn a pump that will filter water to make it potable.

## System Design Overview

This system is designed to take power from a solar panel, amplify its voltage to about 320 VDC, and invert that DC voltage into three-phase AC voltage (Figure 2). Power flow, sensor data and control

signals are represented by the red, blue and green lines, respectively. The main circuit consists of two power stages: DC-DC and DC-AC. The DC-DC stage transforms the DC voltage from the solar panel (18-33V) into a 320 nominal volt DC bus. The DC-AC stage inverts the new DC voltage into three-phase, 220V AC. These three balanced phases are controlled and drive the induction motor. Auxiliary systems, which are isolated from the main circuit, are also powered by the solar panel. The microcontroller processes the data and makes adjustments as necessary to keep the system running and maintain maximum efficiency.

## DC-DC Converter

The DC-DC stage amplifies the DC voltage taken from the solar panel. A full bridge DC-DC converter was chosen as the preferred topology because of its transformer utilization ratio, lower voltage rating for switches, and efficiency (Figure 3). The voltage output is given by Equation 1 in the appendix.

The transformer is supplied with an alternating pulse train from the full bridge. This causes an alternating current in the transformer. A voltage amplification ratio of 18 was needed to amplify the solar panel voltage from 20 VDC to the DC bus voltage of 330V. Equations 2 and 3 were used to determine the number of turns needed on each side of the transformer. Peak current was determined using Equation 4 and the RMS value using Equation 5. Equation 6 gives the

*“Rural areas lack access to stable power and water supplies. Therefore, a viable solution must harness energy from the environment and use it to purify water.”*

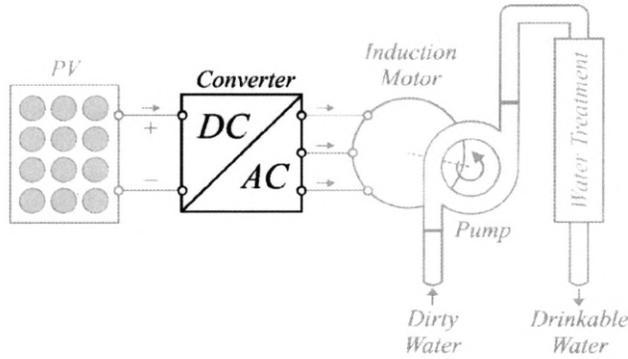


Figure 1. Diagram of a solar panel to clean water system

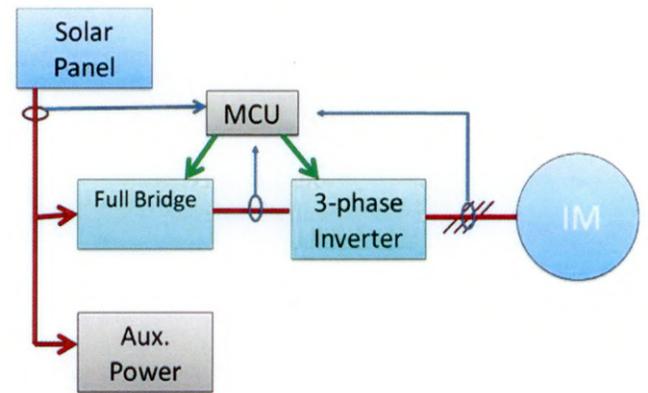


Figure 2. System overview

secondary current, and wire size was determined by Equation 7. All of these factors were included to produce the ideal transformer using a ferrite core.

The inductor in this converter is of great importance, and the design and selection in a full bridge converter is similar to a buck converter. The inductor had to work in Continuous Current Mode over a wide range of power. Equation 8 was used to develop a baseline value for the inductor. This came out to be 16mH. The inductor built was 27mH to reduce ripple current.

The switches used were chosen for their high efficiency. The switching frequency chosen had to maximize efficiency and minimize system cost and size. The converter was designed to operate at 20kHz because of available magnetic cores and designing experience. Testing showed that the maximum efficiency was obtained at 40kHz, which was chosen as the DC-DC operating frequency.

### DC-AC Inverter

The DC-AC Inverter changes the DC voltage into three-phase AC. This three-phase output is what powers the motor. A conventional six-switch, three-phase inverter was chosen for this due to its simplicity and ease of control (Figure 4).

The criteria used for choosing the switches for the inverter were voltage, current rating, and losses. The switching frequency was selected to be 20kHz based on the system power level and the maximum output line voltage.

Sinusoidal Pulse Width Modulation (SPWM) and Space Vector Pulse Width Modulation (SVPWM) were the two options for the modulation method. Conventional SVPWM, however, is equivalent to harmonic injected SPWM, and since SVPWM is more complex in calculating sectors and vector duration, SPWM was chosen because of the relative simplicity of calculations and ease of

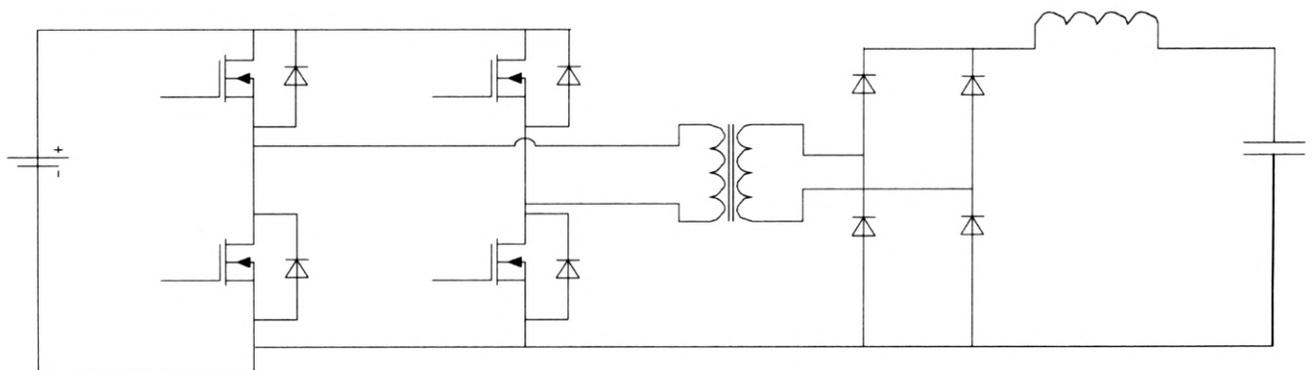


Figure 3. Full bridge topology

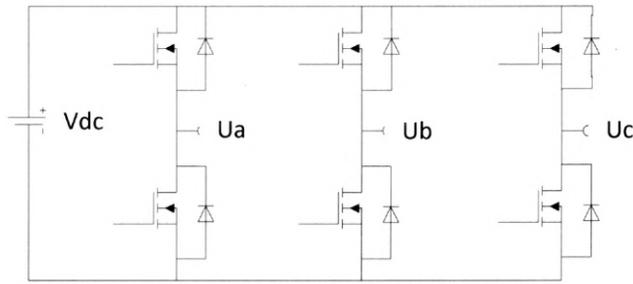


Figure 4. DC-AC inverter topology

understanding. Equations 9, 10 and 11 were used to calculate the duty cycles of phases a, b and c, respectively. From there, a modified SPWM method was used that consolidated the 000 and 111 vectors. This modulation strategy was calculated using Equations 12, 13 and 14. This made the switching time and loss two-thirds of that of the conventional SPWM.

**Motor Drive**

When designating a control method for the induction machine, Field Oriented Control (FOC) and Voltage/Frequency (V/F) control were considered. FOC gives a better dynamic response, but it is more sophisticated and requires additional hardware. V/F was chosen according to the criteria of simplicity, reliability and cost.

Voltage/Frequency control adjusts the motor speed by controlling the stator excitation frequency. The induction machine stator voltage can be described, neglecting the stator resistance and leakage inductance, by Equation 15. The rotor speed is then given by Equation 16. Because the slip ratio is very small under high efficiency conditions, the rotor speed is approximately proportional to the stator excitation frequency. As the motor torque is linear to the magnitude of flux, the stator voltage to frequency ratio has to be constant to maintain the same level of torque during speed control. In reality, the voltage drops across the leakage, and the stator resistance is comparable with the stator voltage at low speeds. Under this situation, compensation is required to improve performance.

**Maximum Power Point Tracking**

Maximum Power Point Tracking (MPPT) allows for the circuit to work at its highest potential. Solar panel output is affected by operation point voltage/current as well as the solar intensity and atmospheric pressure. These factors require a maximum power point tracking method to obtain maximum power from the solar panel. A combination of the Constant Voltage Tracking (CVT) and Perturbation & Observation (P&O) methods was used for this design. CVT is based on the fact that the maximum power point for this system is around a fixed ratio (0.78-0.81) of open circuit voltage. The approximate maximum power can be obtained by setting the solar panel voltage at a fixed value. P&O dynamically disturbs and searches over different operation points

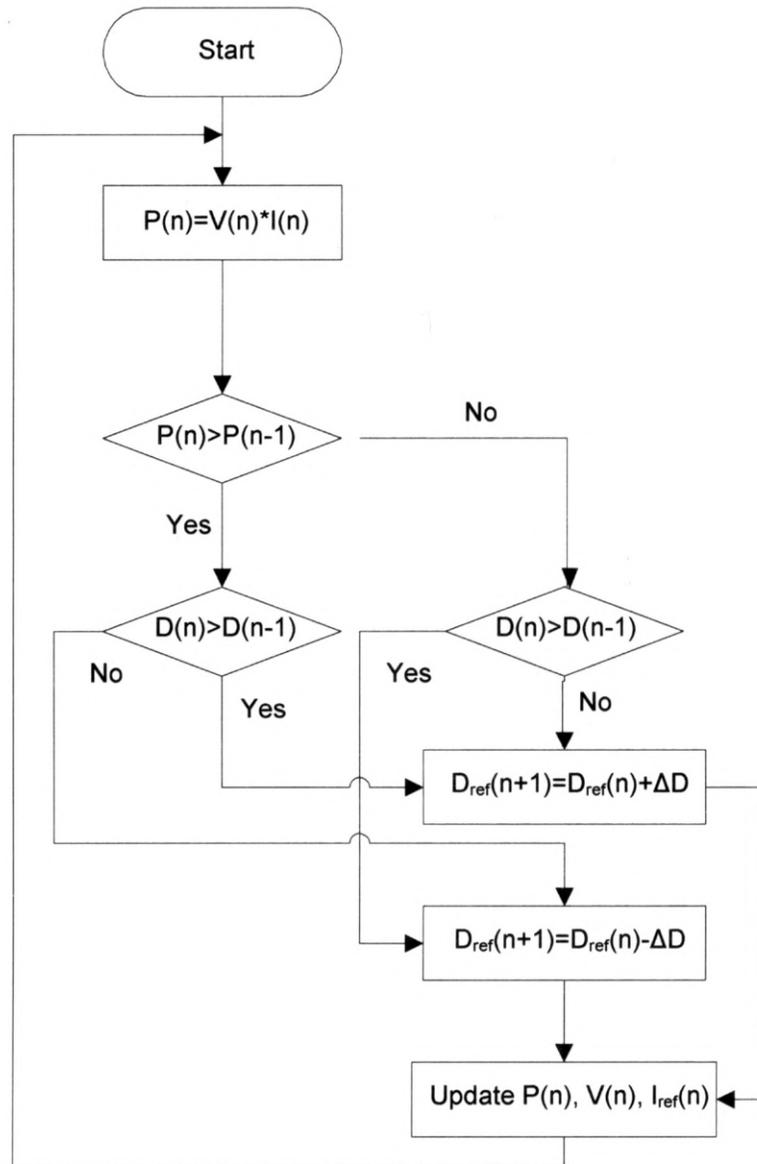


Figure 5. Flow chart for operation of MPPT

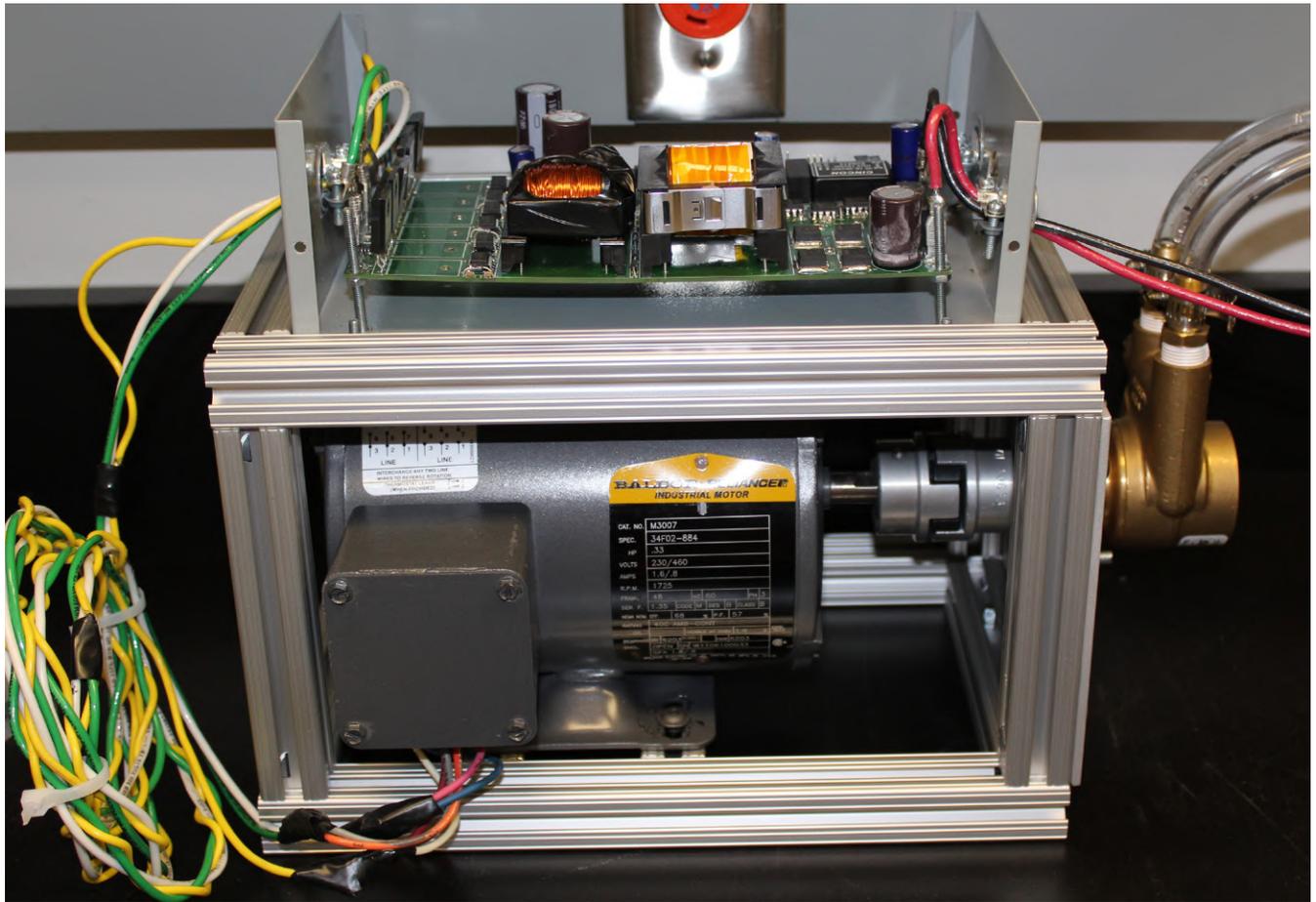


Figure 6. Open view of the system

until it finds a maximum. At startup, CVT brings the system to a point close to the maximum, then P&O takes over to find the exact maximum power point. This allows the system to start up quickly and then search for a more accurate and efficient point. The search step is set at 0.01, and the search period is 1 second (Figure 5).

### Auxiliary Circuits

A signal buffer circuit was needed to protect the microcontroller. If too much heat or current enters the microcontroller, there is a possibility that it will burn and fail. The buffer circuit allowed for protection against destroying the microcontroller. The microcontroller output is buffered to boost the output current capacity and reduce the likelihood of burning the microcontroller. A gate driver circuit for power semiconductor switches was built to provide the voltage and power to turn the switches on and off. Voltage divider circuits are used for voltage sampling, and a Hall Effect sensor is used for panel current measurement.

An auxiliary power supply was used for the

gate drivers, the sampling circuit and the microcontroller. This reduced the risk of burning major components and allowed testing and debugging at lower voltages. This auxiliary circuit also allowed for different standby modes. The system had three modes: Cold Standby, Hot Standby and MPPT. Cold Standby checked if the system control relay was on and if there was water in the tank to be pumped. Hot Standby occurred if the Cold Standby requirements were met, but the panel voltage was below 25V, meaning that the radiation was low and that the solar panel could not provide enough power to start the system. If the Cold Standby requirements were met, and the panel voltage was about 25V, the system would enter MPPT mode and operate until a condition failed to be met.

### Conclusion

Throughout testing, the system performance was averaged over the input power range of 50-200W. The 200-watt operating efficiency was calculated to be 93%, and the average efficiency of the range was calculated at approximately 91%.

The system was effective in pumping water at a high and efficient rate. The system is currently being modified to attain greater efficiency. Future plans include using the basic system for vehicular purposes. This can be adapted by installing solar panels on the roofs of cars and using them to power drivetrains or auxiliary circuits such as HVAC or A/V systems.

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## Appendix - Equations

- (1)  $V_{DCBus} \approx V_{sp} \times \frac{N_s}{N_p} * D$
- (2)  $N_{pmin} = \frac{V_{pmin} D_{max}}{\frac{\pi^2}{2} \times B_{max} \times A_e \times f}$
- (3)  $T = \frac{N_p}{N_s}$
- (4)  $I_p = \frac{P_{in}}{V_{mppt} \times D}$
- (5)  $I_{pRMS} = I_p \times \sqrt{D}$
- (6)  $I_s = \frac{I_p}{T}$
- (7)  $A_{wire} = 1000 \times I_{p,s}$
- (8)  $L_o = \frac{.5V_o}{f * I_{psecond}}$
- (9)  $Duty_a = \frac{V_{a,ref} P_{counter}}{0.5V_{dc} \cdot 2} + \frac{P_{counter}}{2}$
- (10)  $Duty_b = \frac{V_{b,ref} P_{counter}}{0.5V_{dc} \cdot 2} + \frac{P_{counter}}{2}$
- (11)  $Duty_c = \frac{V_{c,ref} P_{counter}}{0.5V_{dc} \cdot 2} + \frac{P_{counter}}{2}$
- (12)  $Duty_a = Duty_a - \text{minimum}\{Duty_a, Duty_b, Duty_c\}$
- (13)  $Duty_b = Duty_b - \text{minimum}\{Duty_a, Duty_b, Duty_c\}$
- (14)  $Duty_c = Duty_c - \text{minimum}\{Duty_a, Duty_b, Duty_c\}$
- (15)  $U_1 \approx E_1 = 4.44 f_1 N_1 K_{N1} \phi_m$
- (16)  $n = \frac{60f_1}{p} (1 - s)$

# Game-based Simulations:

## Using Stories and Gameplay to Create Research-based Education and Training Environments

by Carrie Crossley

**V**ideo games are arguably the most important form of rising media in the 21<sup>st</sup> century.<sup>1</sup> Most consider games to simply be a form of art or entertainment, but as more research is being done in the field of simulations and virtual trainers, games are becoming an increasingly popular and successful tool for education.<sup>2</sup> By utilizing recent advances in the field of Arts and Technology research, such as technology in artificial intelligence, facial and body animation, and motion capture, developers are now able to create extremely realistic virtual environments for educational simulations. These types of developments, which use elements of video games for specific educational and professional training, are known as game-based simulations.

### Research in Virtual Training

Research in virtual training is beneficial for several reasons. Because video games are easily accessible, students are able to download a trainer from almost anywhere in the world at any time. This method of education not only is convenient but also allows companies to avoid large expenses associated with travel, the creation of physical environments, and

hiring actors. Widespread accessibility also creates efficiency and consistency; online simulations “provide ubiquitous and asynchronous educational opportunities for more students in many locations.”<sup>3</sup> With the growing use of mobile technology, the use

of virtual trainers will become even more prominent and convenient.

Current research in the field of virtual training is yielding many revolutionary projects. Dr. Marjorie Zielke, along with her faculty and student colleagues, recently developed

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two games that typify the advantage of video game-based training and education. These two projects – the First Person Cultural Trainer (FPCT) and the Virtual Pediatric Nursing Trainer: Respiratory Disease (VPNT:RD) – have won national and international awards from groups such as the Department of Defense, the National Training and Simulation Association and the International Meeting on Simulation for Health. FPCT is a game-based simulation designed to train United States soldiers in cross-cultural interaction and decision-making within diverse societies. VPNT:RD teaches undergraduate nursing students to follow the correct medical procedures when dealing with infants with

respiratory diseases. Another type of healthcare simulation, currently under development, explores techniques to virtually train physicians and nurses on excellent and effective communication techniques to promote patient safety.

### The Importance of Storytelling and Dialogue

While many different components of game development go into making a game-based simulation, a particularly important and distinctive feature of a virtual trainer is a high level of player immersion. In order for a game-based simulation to seem real and effective, the player must feel like he or she is actually in the game. While technical aspects of a game certainly have an effect on this perception, one key element to successful immersion is a compelling and purpose-driven story. Within the context of a simulation game, a story can provide mechanisms for player interaction, character development, and tracking progress. A good story “can create strong emotional engagement because people come to care about the characters in the simulation.”<sup>4</sup> However, the player cannot simply observe the story unfold;

*“While many different components of game development go into making a game-based simulation, a particularly important and distinctive feature of a virtual trainer is a high level of player immersion.”*

he or she needs to be involved. In order “to build realism and nuance into psychological, behavioral, and social modeling, the user must have the ability to speak ... through natural verbal communication.”<sup>5</sup>

Narrative and dialogue are also important for character development. During game-based simulations, the player spends a large amount of time interacting with virtual non-player characters (NPCs). In order for these characters to be realistic, the player must be able to sense their personality and feelings. “Because virtual humans look and behave like real people, when real people observe virtual humans they expect the characters to exhibit emotion.”<sup>6</sup>

Effective dialogue contributes to the realism of NPCs by providing a key way to virtually express this emotional dimension.

Aspects of storytelling can be used for more than simply immersion. The story element also provides a construct for tracking progress. In order to complete objectives and proceed in the game, the player must converse with NPCs and receive information that is pertinent to solving problems

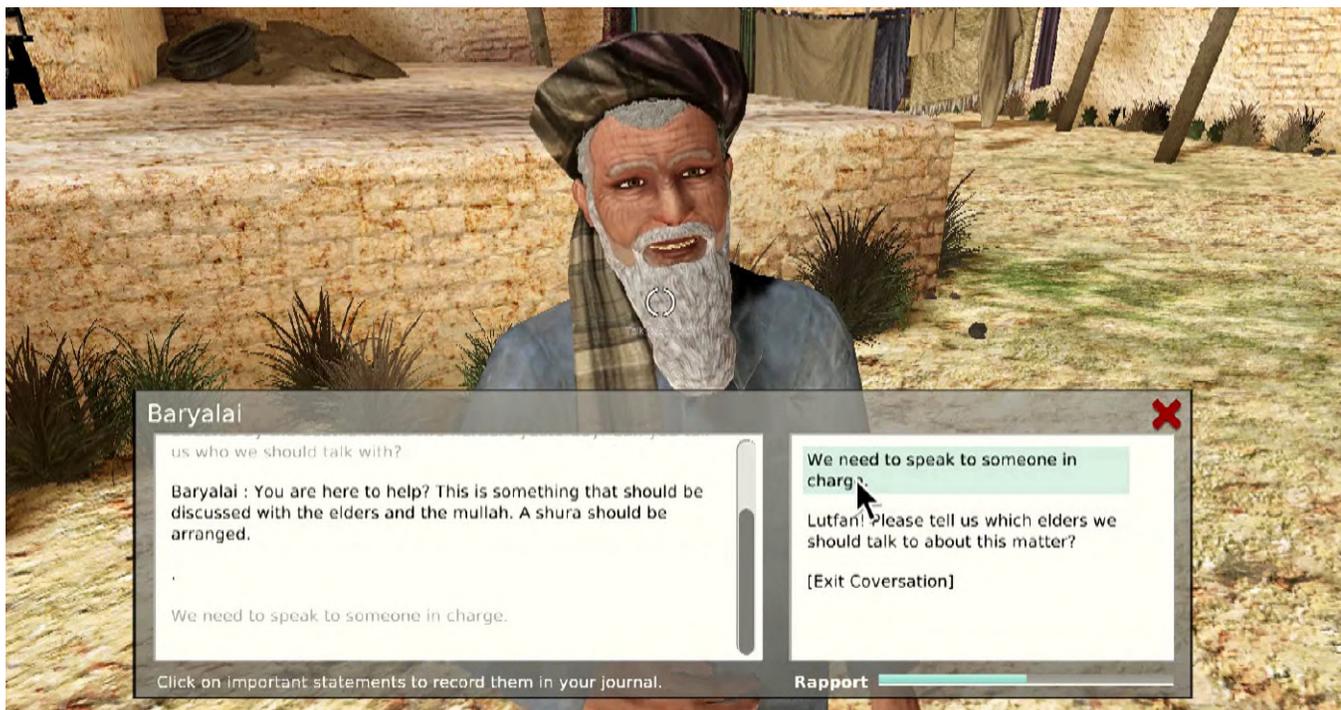


Figure 1. FPCT stresses the importance of proper conversational etiquette by implementing a branching dialogue system. Branching dialogue in FPCT is used to provide a story, enhance character realism, and track the player's progress.



Figure 2. A family is shown interacting with a social worker. Though the player has no personal influence in this scene, he or she is able to read the emotions of NPCs through audio and visual cues.

and continuing the story. “In FPCT, the story is the game ... successful communication with the various NPCs is essential.”<sup>7</sup>

### Dialogue in Gameplay

In order to accomplish realistic communication with story-line characters, FPCT uses a branching dialogue structure, focusing on conversations between the player and various NPCs. Each time an NPC speaks, the player is given three different response options: an optimal reply, an acceptable reply and an unacceptable reply. Accordingly, depending on what responses the player chooses, he or she progresses on the optimal path, the acceptable path or the unacceptable path. Each path sends the player to different NPCs and story branches, allowing the player to obtain different information. Choices made within the interactive story can either help or impede the successful navigation of the game. By choosing different dialogue options, the player can switch paths many times in one game, but he or she is evaluated on every step of the process and not simply the end result.

Other projects from Dr. Zielke’s lab, such as VPNT:RD, incorporate different conversation styles. This approach to dialogue gives the player a lot of freedom, but also allows the developer to keep certain elements of the story static. For ex-

ample, in VPNT:RD the player may interact with a virtual charge nurse after examining a child. Other scenarios feature a social worker speaking with the child’s family. These conversations can involve a wide variety of scenarios and characters, including other types of medical staff, patients and family.

### Conscript™ and How it Facilitates Branching Narrative

Conscript™ is a programming language designed to manage this essential narrative and branching dialogue. Conscript™ is a helpful tool for developers because it is easy to use but has a wide variety of functions. The basic nature of coding in Conscript™ allows writers with little computer programming experience to develop dialogue and assign it to specific characters or situations. Conscript™ is frequently utilized to manage interactions between players and NPCs, as well as between NPCs.

Using Conscript™ allows the developer to associate specific dialogue with different animations, mood influences, and player objectives. Certain conversational responses can affect the emotions of an NPC, and Conscript™ allows these responses to trigger different visual cues for the player. In addition, certain pieces of information acquired in conversation can be tagged as “golden nuggets” and used to track the player’s progress throughout the

game. Conscript™ has the potential to revolutionize virtual training research, because it creates “a conversation system that is dependent not simply on the player selecting the ‘right’ choice, but also on the player’s perception of the attitudes and situations of the people to whom they are talking.”<sup>8</sup>

### The Future of Virtual Trainers

Research in virtual training and simulation is becoming increasingly popular, and knowledge on the subject is growing rapidly. Soon, with the advancement of current technology, developers may be able to produce even more realistic simulations. For example, Dr. Zielke’s lab is in the process of creating Visual Conscript™, an enhancement to Conscript™ that will allow writers to create story components through flowcharts and other visual interfaces. Similarly, as researchers discover more ways to integrate dynamic story and dialogue generation into tools like Visual Conscript™, the use of game-based simulations will likely advance – making realistic, immersive and effective storylines within a game an even more powerful training and education tool.

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Figure 3. This scene incorporates training in both conversational ethics and proper medical procedures. A player interacts with a physician after calling him in on a false alarm.

# Sequencing in the Future: Characterizing the Influenza B Genome by Sanger and Illumina Processes

by Truc K. Do

**W**ith the discovery of the DNA double helix, James D. Watson mused, “Then DNA was still a mystery, up for grabs, and no one was sure who would get it and whether he would deserve it if it proved as exciting as we semisecretly believed.”<sup>1</sup> A few decades later and with the development of massive parallel sequencing technology, DNA has in a sense become less mysterious as genome data are generated at a rate of billions of base pairs each day. At the forefront of the sequencing world is the Genome Sciences Group at Los Alamos National Laboratory (LANL). Nestled in the magnificent Jemez Mountains region, Los Alamos was once home to Project Y of the Manhattan Project but now hosts a consortium of state-of-the-art research facilities: the National High Magnetic Field Laboratory (NHMFL), the Los Alamos Neutron Science Center (LANSCE), the Center for Integrated

Nanotechnologies (CINT), and the Joint Genome Institute (JGI-LANL). As a LANL intern for the past two summers, I worked with high-throughput Sanger and Illumina sequencing pipelines to assemble complete RNA-based genomes of several influenza B viruses.

## High-throughput Sequencing Facilities

The U.S. Department of Energy (DOE) Joint Genome Institute (JGI) is comprised of six facilities across the nation whose mission is to advance the field of genomics for bioenergy and biosecurity-related studies. The six facilities include five national laboratories: Lawrence Berkeley, Lawrence Livermore, Los Alamos, Oak Ridge and Pacific Northwest. The HudsonAlpha Institute for Biotechnology constitutes the sixth branch of JGI. Each branch possesses its own expertise, with Los Alamos leading the way

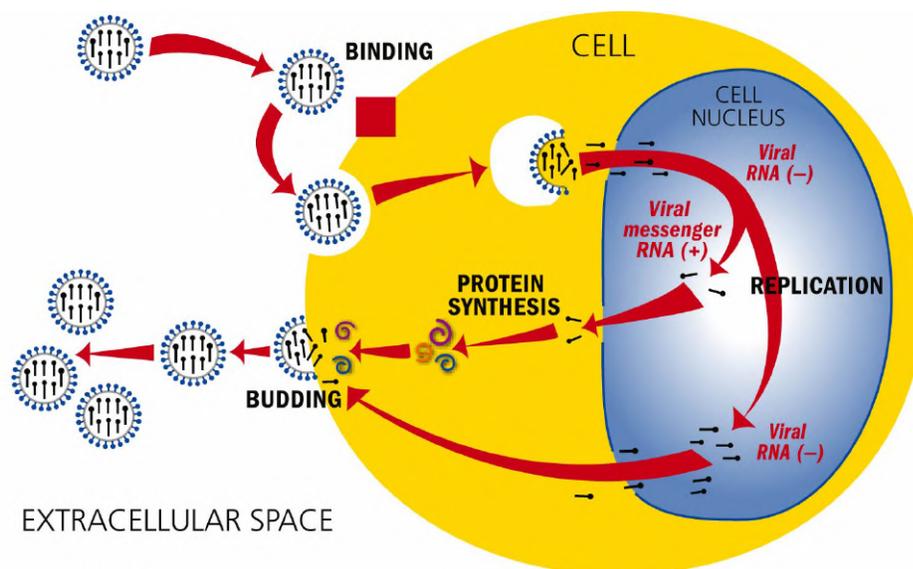


Figure 1. Extracellular space. Courtesy Kathryn Seely, Cornell University

in microbial genome finishing and high-throughput sequencing. As there is increasing use of sequence data in molecular biology and genetic research, there is a demand for faster and cheaper methods to generate accurate data. Los Alamos is at the forefront of mobilizing efforts to close this gap, and among its many cutting-edge projects is the influenza sequence database.

## The Influenza B Virus

The Centers for Disease Control and Prevention (CDC) estimated up to 49,000 flu-related deaths between 1976 and 2006.<sup>2</sup> Each year, billions of dollars are spent on influenza research and vaccine development. Seasonal “flu shots” include inactivated influenza A and B viruses that prepare the body for potential attack. This study examined influenza B viruses, which can undergo gradual antigenic drift (mutation) to accumulate greater virulence.

There are three different types of influenza viruses (A, B, C), each with varying propensity toward infection in human beings.<sup>3</sup> While influenza B is less virulent than influenza A, it can still cause severe respiratory illness and widespread human epidemics.<sup>4</sup> An influenza B virion contains genetic material enveloped by a protein and lipid coat.<sup>5</sup> On the surface of influenza B viruses are two distinct antigenic glycoproteins: hemagglutinin (H) and neuraminidase (N).<sup>6</sup> The hemagglutinin protein is responsible for the cell-surface binding specificity of host-virus interaction and the entry of viral genome into the host cell by membrane fusion upon infection.<sup>7</sup> Viral neuraminidase proteins are necessary for release of progeny influenza viruses from the host cell to infect neighboring cells.<sup>8</sup> Different strains of influenza B show a variety of surface glycoproteins, and with that a diverse host range. Within the capsid of the influenza B virions is a single-stranded, negative-sense RNA genome [(-) ssRNA] divided into eight separate segments.<sup>9</sup> Eleven different proteins essential to viral replication and propagation are encoded by this approximately 14,000-nucleotide-long genome, including the hemagglutinin and neuraminidase surface antigens.<sup>10</sup>

Influenza B shares a similar path of infection with influenza A (Figure 1).<sup>11</sup> Viruses enter by receptor binding of host cells typically found in the lungs and air passages of humans.<sup>12</sup> The released negative-sense RNA genome is made by host cell machinery into positive-strand messenger RNA, which is then translated into viral proteins.<sup>13</sup> Additional copies of (-) ssRNA are made in the host cell nucleus and packaged with these viral proteins to produce progeny virions.<sup>14</sup> Assembled progeny viruses bud from host cells and are released into the extracellular medium for further infection.<sup>15</sup>

By the process of random antigenic drift, influenza B viruses can accumulate significant changes or mutations in its genome over a period of time.<sup>16</sup> The mutations are manifested in expressed viral proteins, particularly hemagglutinin and neuraminidase. This leads to new influenza strains

*“Bioinformaticists and computational biologists can use these sequences to map mutations between different strains of influenza, and thereby monitor the evolution of the virus from year to year.”*

yet unrecognized by the body’s immune system, as there are no antibodies available to defend against the foreign antigens.<sup>17</sup> We sequenced and assembled the complete genomes of different influenza B viruses, which were phylogenetically analyzed to monitor flu outbreaks and develop effective vaccines.

## Method: Sequencing by Synthesis

All sequencing techniques are based on a simple paradigm: whole genomes are broken up, sequenced and finally reassembled. Think of it in terms of a jigsaw puzzle. A jigsaw puzzle is analogous to a whole genome, in this case the genome of a unique influenza B virus. The puzzle (genome) is at first broken up into individual puzzle pieces (genome fragments) and must be reassembled based on overlapping regions to give a complete picture (RNA sequence).

Sanger and Illumina methods were used to sequence influenza B viruses. The high-throughput sequencing pipeline, developed at LANL, is a model to extract, sequence, assemble and publish complete genome data for influenza viruses. After collection and extraction of RNA-based influenza B viruses, the first step in both pipelines was to make double-stranded DNA (dsDNA) from viral RNA since only dsDNA could be sequenced on the platforms. A

one-step reverse-transcriptase polymerase chain reaction (RT-PCR) accomplished this by converting ssRNA to single-stranded complementary DNA (cDNA), which was then amplified up to dsDNA. The degenerate primers used in this reaction were influenza B-specific and produced short 300 to 800 base pair overlapping regions of the whole influenza B genome for downstream (subsequent) sequencing. This RT-PCR step is analogous to breaking up a jigsaw puzzle into separate pieces (overlapping regions) for reassembly. For both pipelines to operate properly, a magnetic bead process was used to clean RT-PCR products and remove contaminants. After cleanup, the dsDNA product was ready for sequencing on either Sanger or Illumina pipelines. This is again analogous to a jigsaw puzzle, where the puzzle pieces (dsDNA fragments) must be organized via downstream systematic pipelines before reassembly.

### Traditional Sanger Sequencing

Sanger sequencing is based on separation by capillary electrophoresis and fluorescent detection of dideoxy-terminated PCR products. Cleaned dsDNA served as a template in the downstream sequencing reaction with the following reagents and components: dideoxynucleotides (ddNTPs), buffer, water, and universal forward and reverse sequencing primers.

The ddNTPs were nucleotides that lacked 3'-OH groups and were covalently coupled to fluorescent labels.<sup>18</sup> Based on a three-step denaturation, primer annealing and primer extension protocol, DNA polymerase enzyme added nucleotides to the 3'-end of a growing DNA strand using the dsDNA template in a 25-cycle reaction.<sup>19</sup> Occasionally, the DNA polymerase added a ddNTP to the growing strand instead of a regular nucleotide. Because ddNTPs lack 3'-OH groups necessary for continuing nucleotide addition to the growing strand, elongation of the DNA strand was terminated. The position of termination was variable, depending on when and where the ddNTPs were incorporated. This sequencing reaction produced many 3'-ddNTP terminated fragments of variable length from the template dsDNA. PCR products were separated by electrophoresis on an Applied Biosystems® 3730xl 96-capillary analyzer. Fluorescent end-labeled PCR products that were terminated early were shorter in length, and so they migrated faster down the capillary. This led to discrete separation of labeled

PCR products that differ by one base pair. As each product migrated down the gel and exited the capillary, it fluoresced according to the identity of its incorporated 3'-ddNTP upon laser excitation.<sup>20</sup> A detector recognized this 4-color fluorescence and differentiated between A, G, C and T nucleotides to give sequence data trace for alignment and assembly.<sup>21</sup>

### Next-generation Illumina Sequencing

The next-generation Illumina method also used cleaned, amplified double-stranded genomic DNA, but followed a different downstream sequencing process consisting of three main steps: (1) sample library preparation, (2) cluster generation and (3) cyclic-array sequencing. Cleaned dsDNA from RT-PCR reactions were adenylated at the 3'-ends by addition of a single "A" nucleotide. In the subsequent adaptor ligation step, short DNA fragments (adaptors) with "T" overhangs were ligated onto the complementary adenylated ends. The products of adenylation and adaptor-ligation were adaptor-flanked double-stranded genomic DNA fragments of approximately 300 to 800 base pairs in length. This size range of flanked template DNA was optimal for sequencing conditions since the Illumina method was size specific. Contaminants and excess reagents were removed from these reactions by the magnetic bead cleanup process. After cleanup, flanked template DNA was PCR-amplified, validated, and pooled into one reaction tube for cluster generation.

Following sample library preparation, the adaptor-flanked DNA template was further amplified by bridge or cluster PCR on the surface of a solid flow-cell substrate to give spatially distinct clonal clusters called "colonies."<sup>22</sup> Forward and reverse primers were covalently attached to the flow-cell surfaces. When flanked DNA template was denatured and added to the flow cell, the single-stranded DNA bound to the surface by complementary base pairing between its ligated adaptor and surface primers. Each region of the flow cell was unique to a single-stranded DNA template, which formed a bridge on the flow cell surface by base pairing with another complementary primer. A DNA polymerase-catalyzed PCR reaction produced millions of "colonies" spatially separated and immobilized on the flow-cell surface.<sup>23</sup> Each "colony" contained ~1000 ssDNA amplicons (copies) of a single DNA template molecule.<sup>24</sup>

Sanger	Illumina
<ul style="list-style-type: none"> <li>• Up to ~800-900 bp read lengths</li> <li>• Per-base 'raw' accuracies as high as 99.999%</li> <li>• \$500 per megabase cost</li> <li>• Finishing reactions with specific primers designed</li> <li>• Shotgun <i>de novo</i> sequencing relies on cloning in <i>E. coli</i></li> <li>• Still most accurate sequencing method (note ghost reads)</li> </ul>	<ul style="list-style-type: none"> <li>• Up to 2 x 100 bp independent reads for paired-end libraries</li> <li>• Per-base 'raw' accuracies from ~98.5-99%</li> <li>• &lt;\$0.01 per megabase cost</li> <li>• <i>In vitro</i> library preparation and clonal amplification</li> <li>• Massive parallel sequencing on microchip technology</li> <li>• Substitution error</li> </ul>

Table 1. Comparison of results from Sanger and Illumina sequencing pipelines. Used in tandem, these pipelines produce comprehensive sequence data for influenza studies. Citation: Michael L. Metzker, "Sequencing technologies - the next generation," Nature Reviews Genetics 11 (January 2010): 37.

Single-stranded amplicons on the flow-cell surface were sequenced on an Illumina® HiSeq 2000 cyclic-array sequencing platform. The Illumina method used "reversible terminators," which were dNTPs with two chemical modifications: (1) 3' chemically cleavable moiety allowing for only single nucleotide incorporation per cycle and (2) one of four chemically cleavable fluorescent labels corresponding to either A, G, C or T nucleotides.<sup>25</sup> During each cycle of a 200-cycle sequencing reaction, a DNA polymerase incorporated a single "reversible terminator" nucleotide to the growing strand at the 3' end according to its DNA template. This extension occurred in parallel fashion across all "colonies." When the chemically cleavable moieties of the reversible terminators were cleaved, fluorescence was emitted.<sup>26</sup> Emission spectra for all array features in parallel were recorded as sequence data, and the next cycle began.

## Results and Discussion

Sequence data were used to optimize Sanger and Illumina processes for high-throughput influenza B sequencing and to determine if next-generation platforms could provide faster and more accurate data. We analyzed the quality of the aligned influenza sequencing reads, searched for strings of sequences, combined complementary contigs, checked for open reading frames, and tagged the beginning and ending sequences of the segmented viral genome (Table 1).<sup>27</sup> Results proved that Sanger

sequencing generated longer and more accurate reads, though at greater costs. The Illumina method produced shorter reads and lower accuracy, but at minimal costs. Efficient and accurate whole genome sequence data from both pipelines will contribute to the development of a real-time global surveillance system for influenza pandemics and treatment. One method would be to use Illumina for *de novo* or draft sequencing, followed by Sanger finishing to close gaps or missing sequences in the genome.

Los Alamos is unique in its approach to assembling a comprehensive influenza sequence database by these high-throughput techniques that are fast, cheap and accurate. Currently, there are few other sequencing facilities in the U.S. with the capability and resources to draft and finish genomes as efficiently.

Now, what can we do with all of this data? Draft influenza sequences can be aligned and analyzed against known sequences from other influenza strains using an online genomic BLAST (Basic Local Alignment Search Tool) database. There are, of course, epidemiological implications here as well. Bioinformaticists and computational biologists can use these sequences to map mutations between different strains of influenza, and thereby monitor the evolution of the virus from year to year. This phylogenetic history of the virus is especially relevant in predicting the prevalent influenza strains and developing effective vaccines during the next influenza season.

## Future Direction of Sequencing: The Bioinformatics Challenge

The automated handling of influenza viruses is a collaborative effort behind the High Throughput Laboratory Network (HTLN) led by LANL in conjunction with UCLA, and can process up to 80 influenza B samples in a 14-hour run. The influenza sequence database project is, however, only one of the many endeavors undertaken at the Joint Genome Institute-Los Alamos. We now face a crucial dilemma in this new age of sequencing. With a flood of sequence data coming off Sanger, Illumina, Ion Torrent, and 454 pyrosequencer platforms daily, the challenge lies less in producing sequences than it does in analyzing and assembling the data.<sup>28</sup> In fact, sequences produced by a robot that takes up minimal space (perhaps less than the size of a small desk for certain platforms) may require terabytes of memory for storage and computation. There is not yet a system in place to streamline the extensive assembly process that follows sequencing. Faced with the new bioinformatics challenge, perhaps we can prevail as we did in 2003 with the completion of the Human Genome Project.<sup>29</sup>

## Acknowledgments

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# Synthesis of Shape Memory Polymer Coatings in Local Sonic Resonators for Acoustic Metamaterials

by Jessie Gonzales

**M**etamaterials are composite materials that absorb electromagnetic, acoustic or elastic waves at resonant frequencies extremely well. Attenuation of acoustic waves at specific frequencies (a bandgap) is achieved when the metamaterial effectively vibrates out of phase with reference to an incoming sonic wave to cancel the sound. In this work, we synthesize acoustic metamaterials consisting of millimeter-sized, coated, dense, metallic spheres embedded in a stiff epoxy matrix. We substitute a standard soft polymer coating with a shape memory polymer (SMP) coating that possesses the ability to change stiffness as a function of temperature. The resulting change in the internal vibrations in the SMP acoustic metamaterial will consequently cause sound

*“An airplane cabin could someday be coated with a material system that self-adjusts to block out unwanted engine noises.”*

waves to be absorbed at a new resonant frequency depending on the temperature of the material. For instance, an airplane cabin could someday be coated with a material system that self-adjusts to block out unwanted engine noises. SMP metamaterials could also be used in defense applications where specific frequencies of sound can be blocked in very thin materials. They also have potential in “smart”

soundproofing of floors, walls, fuselages and machinery.

This study specifically demonstrates a novel process to

synthesize shape memory polymer acoustic metamaterials so that exotic sound manipulating devices can be realized in the future. A thermoplastic resin is first synthesized using atom transfer radical polymerization (ATRP) in order to improve adhesion around the metallic spheres and reduce irreversible shrinkage during subsequent ultraviolet crosslinking. Thermomechanical tests such as Dynamic Mechanical Analysis (DMA) and Differential Scanning Calorimetry (DSC) are used to verify SMP coating properties.

## Introduction

The first theoretical conception of what would come to be called metamaterials dates back to the 1950s when a Russian mathematician, Veselago, first proposed the numeric abnormalities of a medium having both negative permeability and permittivity.<sup>1</sup> His research, published in a Soviet scientific journal, was somewhat forgotten until a team of U.S. scientists in the late 1990s realized his theoretical musings had tangible application in new-age composites

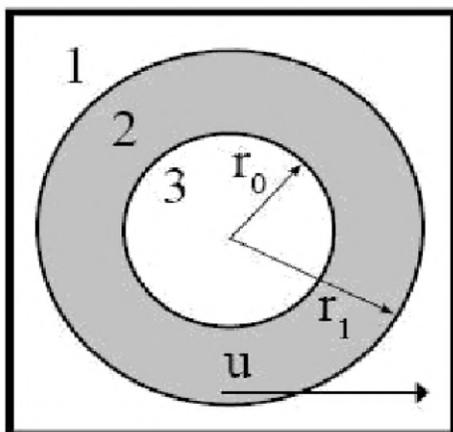


Figure 1. Schematic of a local sonic resonator in an acoustic metamaterial. Regions 1 and 3 represent stiff materials such as epoxy matrix and lead spheres, respectively. Region 2 represents the soft elastomeric coating.

because the wave properties within a composite change, depending on the geometries of the various included materials. The result of this new work became realistic materials having negative indices of refraction relative to vacuum and negative group velocities at resonant frequencies, which led to the development of electromagnetic metamaterials. Experiments by Pendry<sup>2</sup> using split-ring resonators and by Grbic and Eleftheriades<sup>3</sup> using discrete capacitors and inductors demonstrated the double negative parameters of a material. With many researchers and scientists attempting to create various types of metamaterials,<sup>4</sup> Veselago's research had become the cornerstone of metamaterial design. Because wave propagation is extremely similar for most types of waves, researchers began to question (and experimentally verify) whether materials could have negative parameters relative to other forms of waves such as acoustic waves.

Acoustic metamaterials are materials with a negative "effective" mass density and bulk modulus occurring only at resonant frequencies. These artificial materials demonstrate a variety of counterintuitive (and possibly useful) behaviors with respect to the propagation of sound waves through them. They consist of local sonic resonators (coated, dense spheres embedded in an epoxy matrix) as seen in Figure 1. Local sonic resonators attenuate sonic waves at resonant frequencies, determined by the size and density of the embedded metallic sphere and the stiffness of the soft polymer coating. The material is structurally designed in such a way that resonant sound waves traveling through the material will be reflected back and out of phase. This reflected sound wave essentially cancels out the incident wave at resonant frequencies.<sup>5</sup> In theory, acoustic metamaterials, like optical metamaterials, can all be used to create "cloaking," "superlensing" and other exotic wave behaviors.<sup>6</sup> These studies start with an ideal acoustic metamaterial, specified only by its component densities and moduli (related to stiffnesses). The negative "effective" density and modulus model is only a crude approximation of wave propagation through the composite material, but it is a sign of the emergence of band gaps<sup>7</sup> which leads to the exotic noise damping behaviors.

Shape memory polymers (SMPs) have the unique ability to be deformed and fixed into a temporary shape when heated above a particular deformation temperature, such as the glass transition

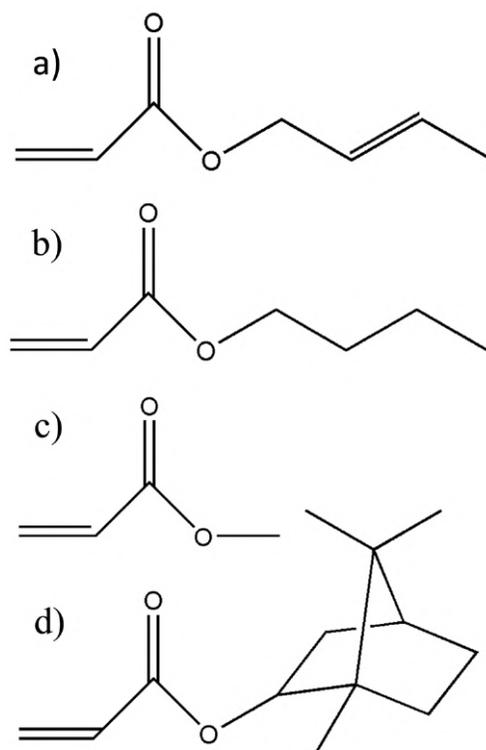


Figure 2. Chemical structure of a) crotyl acrylate, b) butyl acrylate, c) methyl acrylate and d) isobornyl acrylate.

temperature ( $T_g$ ). At  $T_g$ , which varies as a function of chemical structure, a polymer's modulus drops sharply as it enters the rubbery regime.<sup>8</sup> After the polymer is deformed into a new shape by applied stress, and the temperature of the SMP is dropped below its  $T_g$ , the network structure of the SMP will enable it to hold that metastable shape. Subsequent reheating of the material causes shape recovery, up to 800% in certain SMPs.<sup>9</sup>

In this work, we combine temperature sensitive SMPs and acoustic metamaterials. In SMP-based acoustic metamaterials, the bandgap changes as a function of internal temperature because the coating of the local sonic resonator changes in stiffness. We develop a new synthetic approach to fabricate local sonic resonators for SMP acoustic metamaterials.

## Experimental Methods

### Materials

Shape memory polymer coatings are synthesized from the linear monomers crotyl acrylate (CA), butyl acrylate (BA), isobornyl acrylate (IBoA) and methyl acrylate (MA). The crosslinker used is trimethylolpropane triacrylate (TMPTA), and the photoinitiator is 2,2-dimethoxy-2-phenylacetophenone (DMPA). Chemicals to enable atom transfer radical polymerization (ATRP) are ethyl

$\alpha$ -bromoisobutyrate (EBiB), copper (II) chloride ( $\text{CuCl}_2$ ), tris[(2-pyridyl)methyl]amine (TPMA), and tin (II) 2-ethylhexanoate ( $\text{Sn}(\text{EH})_2$ ). The solvent used for ATRP is anisole.

### Synthesis

We synthesize linear copolymers with varying concentrations of the acrylic monomers CA, BA, MA and IBoA pictured in Figure 2. The thermoplastic precursors are synthesized using atom transfer radical polymerization (ATRP)<sup>10</sup> in order to improve adhesion and reduce irreversible shrinkage during subsequent ultraviolet crosslinking around the metallic spheres. The key components in ATRP are the monomers, initiator (EBiB), catalyst ( $\text{CuCl}_2$ ), and ligand (TPMA). The molar ratios of these components control the polymerization kinetics, degree of polymerization, and polydispersity of the resulting polymer. Additionally, excess reducing agent (Sn(II)) is used in order to carry out activators regenerated by electron transfer (ARGET) ATRP.

All of the chemicals are combined in a 20 mL vial, sealed with Durafilm, and polymerized for 8 hours at 75°C. Samples are removed at two-hour intervals for testing by gel permeation chromatography (GPC). Following synthesis, the thermoplastic precursor is combined with varying amounts of TMPTA, a tri-functional monomer, and crosslinked under 365nm UV radiation with DMPA as the photoinitiator. Samples for dynamic mechanical analysis (DMA) and composition selection are polymerized between 75mm x 51mm glass slides and then cut into approximately 3mm x 3mm x 2.4mm samples using a  $\text{CO}_2$

laser cutter.

### DMA

In DMA, an oscillating force is applied to a sample while it is heated. From the force and displacement measurements, the modulus of the material can be determined as a function of temperature and frequency. The  $T_g$  can also be determined from the peak of the tan delta curve at 1Hz. In this study,

*“SMP acoustic metamaterials have the potential to provide greater versatility in terms of shifting frequency bandgaps, thereby creating materials that absorb acoustic waves at different frequencies as a function of temperature.”*

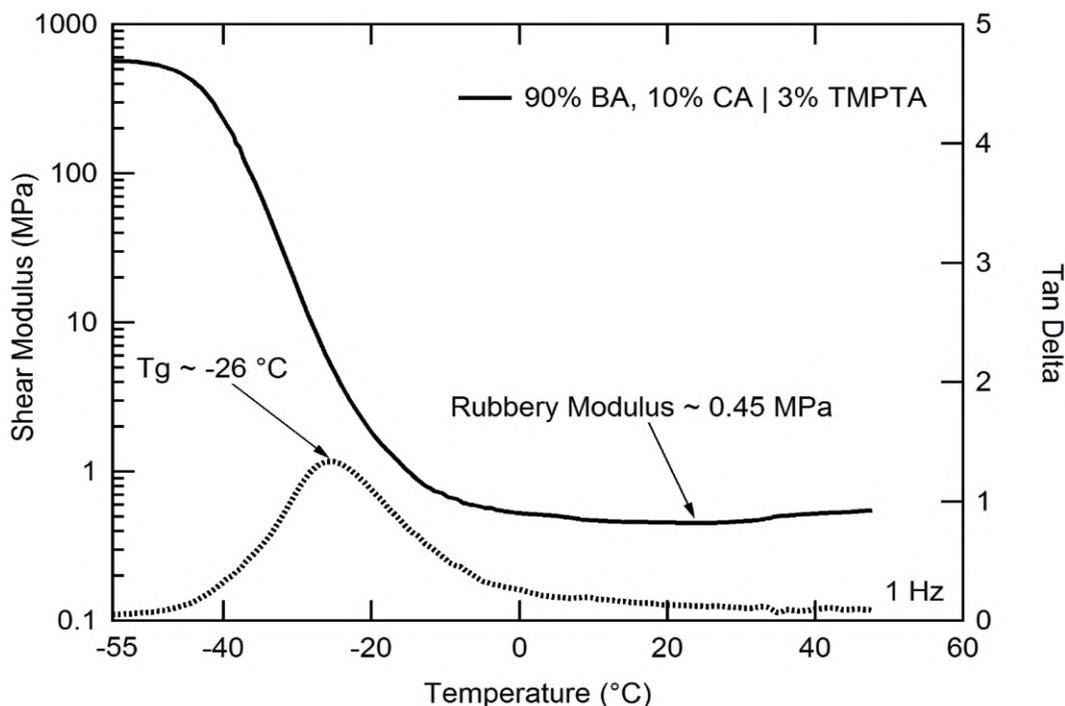


Figure 3. Representative dynamic mechanical analysis curve at 1 Hz for an SMP (A1-3%) made from 90% butyl acrylate monomer and 10% crotyl acrylate monomer and subsequently crosslinked with 3% TMPTA.

samples are tested in shear mode at 1Hz, 2Hz, 5Hz, and 10Hz, to determine the rubbery modulus and  $T_g$ .

## Results and Discussion

In order to understand the effects of acoustic waves on SMP metamaterials and confirm model predictions, several SMP compositions are explored to optimize properties. Figure 3 is a representative DMA curve that highlights the three orders-of-magnitude change in stiffness (proportional to shear modulus) as a function of temperature for a sample made with 90% BA and 10% CA that is subsequently crosslinked with 3% TMPTA and 0.5% DMPA. The shear modulus drops from above 500 MPa in the glassy regime to below 1 MPa in the rubbery regime when measured at 1Hz. The tan delta, plotted on the right axis, peaks at the  $T_g$  and is a visual indicator of the sharp drop in modulus. The rubbery plateau is proportional to the force with which the SMP recovers. Thus the material behaves very differently mechanically at different temperatures. Similar curves for other compositions are examined and data are collected in Tables 1 and 2. Table 1 indicates the shear modulus in the rubbery regime of several polymer compositions while Table 2 plots the  $T_g$  for those compositions.

In the case of the samples A1 to A10, the rubbery modulus and  $T_g$  increase with increasing crosslinker (TMPTA) density and increasing CA concentration. The latter is due to the pendant vinyl bond in crotyl acrylate, which contributes to additional network formation and thus increases the rubbery modulus. It is necessary to be able to independently tune these properties to have full control

Sample	Butyl	Crotyl	Shear Modulus @ Rubbery Plateau (MPa)				
			TMPTA				
			1%	2%	3%	5%	10%
A1	90%	10%	0.33	-	0.45	0.60	1.47
A2	80%	20%	0.52	-	0.65	0.87	1.75
A3	70%	30%	0.46	0.59	0.66	0.80	1.86
A4	60%	40%	-	-	-	1.18	-
A5	50%	50%	-	-	0.91	-	-
A6	40%	60%	0.66	-	1.20	-	-
A7	30%	70%	-	-	-	1.64	-
A8	20%	80%	-	1.17	-	-	-
A9	10%	90%	1.18	-	-	-	-
A10	0%	100%	-	-	2.01	-	5.40

Table 1. Effect of CA and TMPTA on rubbery modulus

Sample	Butyl	Crotyl	Glass Transition Temperature ( $^{\circ}$ C)				
			TMPTA				
			1%	2%	3%	5%	10%
A1	90%	10%	-32	-	-26	-21	-11
A2	80%	20%	-26	-	-24	-18	-14
A3	70%	30%	-24	-23	-23	-18	-7
A4	60%	40%	-	-	-	-12	-
A5	50%	50%	-	-	-14	-	-
A6	40%	60%	-16	-	-11	-	-
A7	30%	70%	-	-	-	-4	-
A8	20%	80%	-	-5	-	-	-
A9	10%	90%	0	-	-	-	-
A10	0%	100%	-	-	2	-	18

Table 2. Effect of CA and TMPTA on  $T_g$

Sample	Linear Monomer Fraction				Additives		Results		
	CA	BA	MA	IBoA	TMPTA	PI	DSC $T_g$ ( $^{\circ}$ C)	DMA $T_g$ ( $^{\circ}$ C)	DMA Er (MPa)
B1	10%		90%		1%	0.5%	14	18	0.38
B2	10%	45%		45%	1%	0.5%	-1	11	0.34
B3	10%	10%	80%		1%	0.5%	7	13	0.42
B4	10%		80%	10%	1%	0.5%	17	22	0.28
B5	10%	30%		60%	1%	0.5%	15	29	0.35

Table 3. Effect of linear monomers on thermomechanics

of the design of local sonic resonators to enable SMP acoustic metamaterials. Thus Table 3 shows how by changing the composition and concentration of linear monomers, we can adjust the glass transition temperature independently from the crosslinker concentration. The concentration of CA and TMPTA can be set to tailor the rubbery modulus, while the ratio of BA, MA and IBoA can be altered to control the  $T_g$ . Specifically, Table 3 shows several compositions with similar  $T_g$  and rubbery moduli with different concentrations of linear monomers.

The polymers made in Table 3 were polymerized directly from the monomers without ATRP in a standard free radical chain growth procedure.

Sample B5 was selected as a viable coating candidate and then made using ATRP instead of by free radical chain growth as in Table 3. Figure 4 shows the change in molecular weight when aliquots are taken from the ATRP reaction in the various compositions at 2 hour time points during the 8 hour reaction.

Figure 5 is a predictive model of the effects of a local sonic resonator on an incident plane wave. The simulation is based on in-house MATLAB programs of a sound plane wave propagating through empty space and an acoustic metamaterial. The simulation demonstrates how the plane wave travels easily through space void of a solid medium (left), while the wave is disrupted and attenuated in the direction of the SMP acoustic metamaterial (right). Absence of a red gradient surrounding the local sonic resonator confirms the theoretical acoustic damping phenomenon.

After the characterization of the various selected compositions, several optimized samples (A1-1%, A2-5%, A3-10% and B5-1%) were chosen to fabricate the first experimental versions of the SMP acoustic metamaterials for testing in an impedance tube. The SMP coating was synthesized around 10mm lead spheres using ATRP to create the thermoplastic precursor. The precursor still contained CA with unreacted vinyl bonds on side chains that were subsequently crosslinked around the lead spheres with TMPTA in an additional UV photopolymerization. This reaction led to several problems including control of reaction kinetics to avoid extreme heating and cracking during the coating process. ATRP oligomers were used to reduce the stresses induced by shrinkage during polymerization, but several samples still cracked when they were coated in larger thicknesses, limiting the truly independent control of thermomechanical properties in the ranges shown in Tables 1, 2 and 3. Figure 6 pictures sample A1-1% cured around 10mm lead spheres and embedded into an epoxy cylinder made to fit inside a two-inch diameter impedance tube.

Additional acoustic testing and optimization will continue to prove the efficacy of these polymer systems for SMP acoustic metamaterials. Further research is also needed to explore improvements to the interface layers between the SMP, metallic

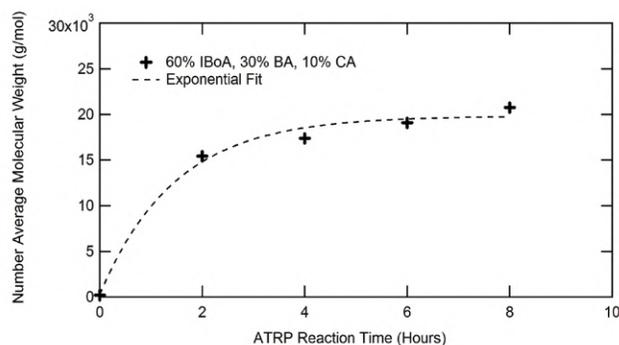


Figure 4. Number average molecular weight at time points during the ATRP reaction of sample B5 as measured by GPC.

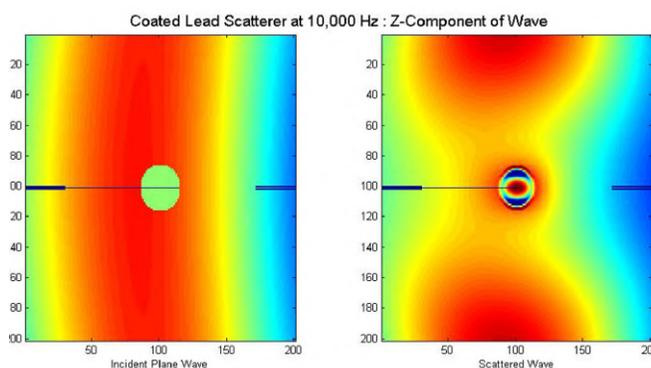


Figure 5. Two simulations describing the effect of a sound plane wave propagating through empty space (left) and through an ideal SMP-based acoustic metamaterial (right). The sound plane wave is represented as the red color gradient with red as peaks and dark blue as troughs.

element and epoxy. The interface cohesion is what allows the device as a whole to vibrate properly for desired sound attenuation. This paper demonstrates a new fundamental technique to post-crosslink oligomers with pendant vinyl bonds in side chains into an SMP coating to enable new paradigms in the design of acoustic metamaterials.

## Conclusion

SMP coatings in local sonic resonators were optimized and synthesized based on predictions from simulations. To accommodate curing around lead spheres, a novel synthetic process is demonstrated, based on copolymerizing linear acrylates using ATRP into short chain polymers and subsequently crosslinking them with TMPTA and UV photopolymerization. Rubbery modulus and  $T_g$  are tuned by varying the composition of linear monomers and crosslinker concentration. We demonstrate the ability to control the coating thermomechanical properties to enable a new class of materials. SMP

acoustic metamaterials have the potential to provide greater versatility in terms of shifting frequency bandgaps, thereby creating materials that absorb acoustic waves at different frequencies as a function of temperature.

### Acknowledgments

I would like to acknowledge the support and guidance of my mentor, Dr. Walter Voit, assistant professor of material science and engineering at UT Dallas. I am very thankful for the endless amount of academic opportunities he has given me. His gracious wisdom and encouragement has positively impacted my undergraduate career as well as my future academic endeavors. I also must thank my colleagues, Brayden Ware, Connie Manz and Vijay Vasan, whose knowledge and expertise were invaluable to the research project. Ultimately, this project would not have been possible without my fellow colleagues and especially not without Dr. Voit.

I also would like to acknowledge my loving family for their abundant support, encouragement and patience in my undergraduate career.

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Figure 6. First experimental version of the SMP acoustic metamaterial. The lead spheres are embedded in a CA-BA copolymer which is in turn embedded into a stiff epoxy matrix.

# When Is Inequality Fair?

by Tanushree Jhunjhunwala

Inequality in income distribution has been a highly debated issue in recent policy discussions in the United States, and in many economies of the world. In order to justify or criticize the prevalence of inequality, we first need to delve into what causes it. We believe factors like sources of income, beliefs about fairness, and the role of chance in economic outcomes greatly impact peoples' preferences about the proper distribution of income.

We conduct a laboratory experiment to investigate factors affecting preferences for redistribution. Our experiment measures how people vote to redistribute a set amount of money from high earners to low earners, depending on how the income is generated. Subjects are placed in high or low income categories through a series of real-effort tasks. In this paper, we attempt to explain the level of inequality that is considered fair among our subject pool on the basis of effort tasks that generate income distributions by chance, skill, speed, intelligence and creativity, as well as a transparently unfair allocation mechanism. Other factors impacting redistribution preferences studied in this paper are personal beliefs regarding altruism and government policies, and individual characteristics such as gender.

## Experimental Design

The experiment is a within-subjects design, where each subject completes decisions for six different

tasks that determine six different sources of income. The subjects complete instructions for each task, and then practice each task for 30 seconds prior to voting on the maximum redistribution amount. After the vote, but before knowing the result of the vote, they complete the task. After completing all tasks, one of the tasks is selected randomly for payment. Throughout the experiment, the subjects earn experimental dollars, which are later converted into U.S. dollars, at a rate of E\$5=US\$1.

For every task, each subject is classified in one of the two income level categories. Out of the twelve subjects in each task, the six that performed the best (except in the luck and unfair treatments explained below) are categorized as high earners and receive 100 experimental dollars. The other six subjects are classified as low earners and receive 20 experimental dollars.

Each subject then "votes" on the maximum acceptable amount they believe should be redistributed from the high to the low earners. The maximum redistribution indicated by the median voter is implemented. The amount chosen is then taken from the high earners and redistributed to low earners.

The first task is based on luck, where the subjects draw a poker chip (with an equal chance of picking either a red chip or a blue chip at the start of the experiment) out of a bag. If this task is chosen for payment, the experimenter asks a subject to draw a

*"The belief that income equality is the responsibility of the government and the subjects' responses to survey questions regarding willingness to help others result in different distribution amounts."*

Variable	Both Genders (N=72)				Males (N=38)				Females (N=34)			
	Mean	Std. Dev.	Min	Max	Mean	Std. Dev.	Min	Max	Mean	Std. Dev.	Min	Max
Luck	32.33	19.02	0	100	34.16	22.9	0	100	30.29	13.48	0	50
Unfairness	31.63	18.85	0	100	30.39	19.68	0	100	33	18.06	0	100
Dexterity	33.36	20.13	0	100	30.92	23.91	0	100	36.09	14.71	0	70
Speed	29.5	22.98	0	100	25.84	26.14	0	100	33.59	18.37	0	100
Knowledge	28.6	20.41	0	80	22.58	21.81	0	80	35.32	16.57	0	80
Creativity	28.69	20.09	0	80	24	21.46	0	70	33.94	17.27	0	80
Total	184.11	121.47	0	560	167.89	135.91	0	550	202.24	98.45	0	480

Table 1. Summary statistics

chip from another bag containing one blue and one red chip. The chip drawn is matched with the chip held by the subjects. Those who hold the same color of chip are the high earners, and the others are the low earners.

The second task measures the effect of an unfair allocation on willingness to redistribute income. The shortest six subjects are the high earners, and the tallest six are the low earners.

The third task is a “slider game,” testing dexterity and mouse control.<sup>1</sup> In this task, 43 short lines appear on each subject’s computer screen. Each line has a tab on it, and the subject needs to bring the tab exactly to 50 by using the mouse.

In the fourth task, the subjects have to add five two-digit numbers displayed horizontally.<sup>2</sup> They are given 120 seconds to complete twelve such sets of numbers. They may use scrap paper but not a calculator. This measures speed and sharpness of mind.

In the fifth task, the subjects answer a set of ten trivia questions in 120 seconds. This is an attempt to study redistribution patterns where income depends on general knowledge and intelligence quotient.

The sixth task is the Remote Associates Test (RAT), devised by Mednick and Mednick, where the subjects are given ten sets of three words. They have to add another word to the three base words to create entirely new words or phrases. For example, adding “star” to “falling,” “actor” and “dust” produces “falling star” “star actor” and “stardust.”<sup>3</sup> This treatment studies willingness to redistribute income based on a process that involves creativity.

After the subjects perform these tasks, only one of the tasks is selected for payment by means of random draw. The subjects then complete a survey and are paid. This procedure ensures that the subjects have an incentive to earn money in each task, without portfolio effects.

Our hypothesis in designing this experiment is that subjects will vote for a higher level of redistribution when income is generated unfairly. Subjects who are sensitive to an unfair distribution of income are more likely to vote for redistribution, even if they expect to do well. Thus our hypothesis is that income redistribution will be greatest for the tasks measuring luck and unfairness followed by tasks measuring dexterity, creativity, speed and intelligence.

## Results

We employ linear regression in order to understand the predictive ability of all the exogenous factors of primary interest: the chief characteristic of each income earning task, gender, views on the responsibility of the government, and an individual’s altruism level. Income equality would have been achieved only if each individual voted for E\$40 making the high and the low earners earn \$17, the average payment. The redistribution amount ranged from E\$0-E\$100 in the first four tasks and E\$0-E\$80 in the last two tasks (Table 1).

Table 2 displays six regression models where each task is the dependent variable. The independent variables are derived from a survey the subjects completed after finishing all six tasks:

- Age – The reported age of subjects.
- Income – The reported income of the subjects.
- Male – A dummy variable where 0=female and 1=male.
- Altruism – An additive variable based on responses to survey questions regarding beliefs in altruism.
- Altruistic Behavior – An additive variable based on responses to survey questions regarding past altruistic behavior.
- Individual Responsibility – A dummy variable

measuring greater agreement with the statement “People should take more responsibility to provide for themselves” than with the statement “The government should take more responsibility to ensure that everyone is provided for.”

- Others versus Self – A dummy variable indicating measuring inclination to “focus on self and family” than to “donate a great deal to others”.

The redistribution amounts of men vary significantly by task compared to that of women (Table 1). Even though the maximum amount redistributed by males is higher in most tasks, the mean redistribution amount of women is higher than that of men. The mean amount under “Both Genders” column shows that people voted for greater redistribution in the tasks which were dependent more on luck or an unfamiliar skill whereas they voted for less distribution for those which tested their intelligence.

Table 2 shows changes in the dependent variable with respect to changes in the independent variables and their associated statistical significance. With respect to gender, we hypothesize that women are more altruistic and should therefore vote to redistribute more. The results confirm our hypothesis as all statistically significant coefficients are negative in the regression outputs. With male subjects, the redistribution amount will decrease by 10.6 units, 11.6 units and 10.5 units in tasks testing speed, intelligence and creativity, respectively.

For the variable Individual Responsibility we hypothesize that people who hold the government responsible to provide for citizens should contribute more. We observe this only in the task measuring intelligence. If subjects believe that people are responsible to provide for themselves, then the redistribution amount is lower by 10.8 units, which is statistically significant. Surprisingly, the coefficients for two of the other tasks are positive.

For Others versus Self variable, we hypothesize that those who donate time or money will redistribute more. Thus, we expect a negative correlation with redistribution. Surprisingly, the regression table shows that as people become more self-centered, their redistribution amount increases, although the coefficient is statistically significant in only one task.

The variables Altruism and Altruistic Behavior are two measures of altruism. The difference between the two is that Altruism is derived from attitude whereas Altruistic Behavior is derived from self-reported behavior. The reason for Altruism to be more statistically significant than Altruistic behavior could be that in the former, people take more leeway in assuming the ways in which they express their altruism in whereas in the latter, due to the directness and specificity of questions, the results indicate that the subjects are altruistic but only in certain aspects and only to an extent.

Tasks measuring speed and knowledge are the

	Dependent variable = maximum redistribution amount by task					
	Luck	Unfairness	Dexterity	Speed	Knowledge	Creativity
Constant	18.741 -0.409	34.855 -0.202	<b>61.259</b> <b>(0.037)**</b>	-23.175 -0.452	26.79 -0.328	11.377 -0.657
Age	0.509 -0.452	-0.273 -0.807	-0.528 -0.657	1.128 -0.374	0.841 -0.454	0.218 -0.782
Male	3.765 -0.365	-3.119 -0.519	-5.382 -0.297	<b>-10.609</b> <b>(0.056)*</b>	<b>-11.617</b> <b>(0.019)**</b>	<b>-10.476</b> <b>(0.024)**</b>
Income	-1.67 -0.507	0.346 -0.912	-1.63 -0.624	-3.37 -0.343	-1.309 -0.677	0.555 -0.849
Altruism	0.094 -0.985	2.205 -0.552	-3.554 -0.369	<b>9.434</b> <b>(0.028)**</b>	-1.742 -0.64	3.048 -0.439
Altruistic Behavior	0.419 -0.598	0.779 -0.841	-2.332 -0.574	5.032 -0.257	1.511 -0.7	4.733 -0.333
Individual Responsibility	2.529 -0.353	-7.858 -0.111	2.628 -0.613	-3.832 -0.49	<b>-10.824</b> <b>(0.031)**</b>	-5.909 -0.222
Others versus Self	4.404 -0.409	-1.173 -0.811	4.676 -0.37	<b>14.084</b> <b>(0.013)**</b>	1.548 -0.753	2.676 -0.603
R-Squared	0.0313	0.051	0.059	0.179	0.182	0.097
Adj. R-Squared	Robust, otherwise -0.075	-0.053	-0.044	0.089	0.092	Robust, otherwise -0.002

Table 2. Regression outputs (OLS, bold indicates statistical significance). All P-values are in brackets.

\*\*P-values significant at 5% \*P-values significant at 10%

only tasks where income is based on skills that are built over time. The subjects are mainly those who have been familiar with addition from a very young age, and IQ builds over one's lifetime. Thus, familiarity with their own capabilities may have guided their redistribution amount better, which results in high adjusted R-squared in these two tasks' models.

On the other hand, the subjects have no control over the tasks that measure luck and unfairness. The dexterity task requires subjects to become adept with the mouse instantaneously, whereas the creativity task requires subjects to come up with insightful answers spontaneously. These two tasks require instant adjustment and wiring of the brain to behave in a certain manner. Thus, the infrequent use of these skills in daily life may affect the redistribution amounts.

The results show that women exhibit stronger preferences toward equity when compared to men with respect to certain tasks. By means of the chi2 test, Table 3 indicates that there is no statistically significant relationship between the first three tasks and gender. However, there is a statistically significant relationship between the two variables at the 10% level for the fourth task and at the 5% level for the fifth and the sixth tasks. Thus, gender has an impact on redistribution amount when sources of income differ as well as when they do not.

## Conclusion

In this paper, we investigate whether peoples' choices involving redistribution of income are altered by the tasks they perform to earn income. We also investigate the effect of personal beliefs on various topics. The belief that income equality is the responsibility of the government and the subjects' responses to survey questions regarding willingness to help others result in different distribution amounts. Gender also has a significant effect on redistribution amounts; we found that females were more altruistic than males and therefore redistributing more.

This experiment concludes that differences in opinion about income inequality can be understood on the basis of personal beliefs and gender. However, sources of income do not substantially change redistribution amounts. We observe significant differences in redistribution amounts in tasks that were familiar to subjects, like addition of numbers and trivia quiz.

Two-way interactions	P-values
Red_chip X gender	0.645
Red_height X gender	0.655
Red_slider X gender	0.397
Red_math X gender	<b>0.081*</b>
Red_quiz X gender	<b>0.012**</b>
Red_rat X gender	<b>0.005**</b>

Table 3. Chi2 test for interactions

\* Significant at 10% level \*\*Significant at 5% level

We intend to improve our experiment by extracting a parameter of self-assessment from the participants of their performance in practice rounds of each task. This will give researchers a stronger data set to evaluate the relationship between confidence and redistribution levels. Understanding a subject's confidence level can foster a better understanding of how people regard the source of income and fairness of inequality.

## Acknowledgments

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# Design Modifications of Reversible Cyclic Peptides for Improved Carbon Nanotubes Dispersions: A Molecular Modeling Approach

by Triet S. Nguyen

Many recent advances in cancer therapy are intimately bound to the use of single-walled carbon nanotubes (SWNTs). As drug carriers, SWNTs are capable of delivering high doses of drugs to specific tumor targets without causing damage to healthy tissue.<sup>1</sup> Concurrently, thermal destruction of cancer cells can be achieved by taking advantage of the near-infrared light absorption property of SWNTs.<sup>2</sup> In addition to cancer therapy, SWNTs have been employed in diverse fields, including materials science,<sup>3</sup> electronics<sup>4</sup> and biotechnology.<sup>5</sup> These applications stem from the excellent mechanical,<sup>6</sup> optical and electrical properties<sup>7</sup> of SWNTs. This is a result of their unique structure: a nano-scaled

cylinder formed from a rolled-up single-layer graphene sheet.

## SWNTs Must Be Made Water-Soluble

The potential of SWNTs in biotechnology, however, has yet to be fully realized due to their intrinsic hydrophobicity, or tendency to repel water. Composed purely of graphitic carbon, SWNTs readily aggregate to form insoluble bundles in an aqueous solution. For most applications, these bundles need to be separated into individual cylinders, which can then stay suspended in the aqueous solution in a manner similar to how pigment is suspended in paint or globules of protein and fat are suspended in milk.

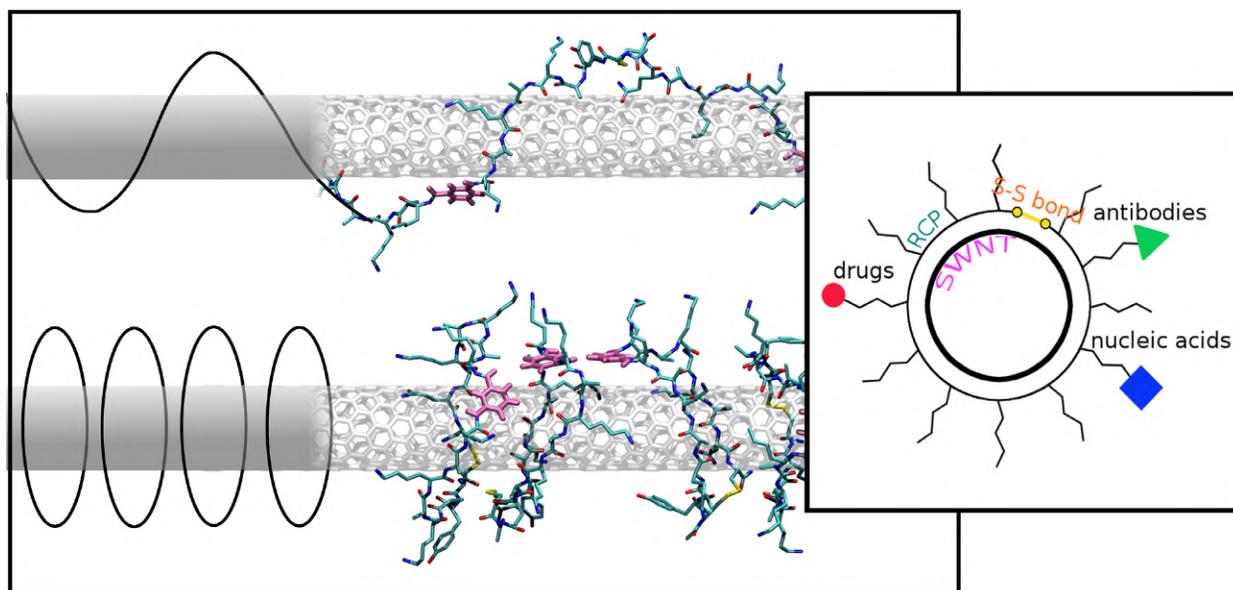


Figure 1. Proposed macromolecular arrangements of multiple RCPs interacting with a SWNT: Polymerized RCPs formed by interpeptide disulfide [S-S] bonds twist around the SWNT (top left), Peptides are cyclized on the SWNT through intrapeptide disulfide bonds and these “rings” stack closely together (bottom left); RCPs are a promising carrier for biomolecules (right).

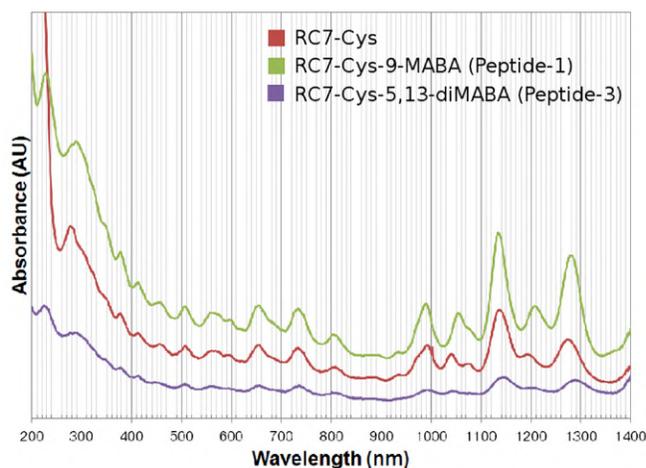


Figure 2. The ultraviolet - visible - near-infrared spectra of SWNTs wrapped with RC7-Cys, Peptide-1 and Peptide-3. The well-resolved peaks and high absorbance of the Peptide-1/SWNT system indicate a significantly higher concentration of singly-dispersed SWNTs compared to the RC7-Cys/SWNT system. The Peptide-3/SWNT spectrum suggests a decreased SWNT dispersion ability for Peptide-3.

This separation can be achieved through either covalent or noncovalent modification of the SWNTs. The covalent strategy<sup>8</sup> involves chemically attaching (bond forming) functional groups to the SWNT sidewalls, whereas the noncovalent strategy utilizes nonbonded interactions of DNA,<sup>9</sup> proteins,<sup>10</sup> peptides<sup>11</sup> or detergents<sup>12</sup> with the SWNT surface. For example, detergents can solubilize SWNTs in exactly the same way that they solubilize oil and dirt particles to clean dishes.

### Reversible Cyclic Peptides as a Solution

Reversible cyclic peptides (RCPs) are well suited for these purposes. Utilizing a noncovalent scheme of SWNT dispersion, UT Dallas chemistry professor Dieckmann and coworkers previously designed and synthesized a series of RCPs<sup>13</sup> that were shown to effectively disperse SWNTs in an aqueous solution. Through controllable solution conditions, a disulfide bond between terminal cysteine amino acids can be formed or broken to give a cyclic or linear peptide, respectively. The disulfide bond (yellow) is shown in the right-hand panel of Figure 1. The peptides coat the surface of individual SWNTs through a combination of nonbonded van der Waals\* (vdW) interactions and the hydrophobic effect, thus shield-

ing individual SWNTs from water and preventing reformation of insoluble aggregates. The primary structural feature of RCPs is that their sequence is comprised of amino acids of alternating chirality.\* Their side chains point radially outward when cyclized around a nanotube, which accommodates the covalent attachment of molecules to the side chains without affecting their SWNT-dispersing ability (Figure 1, right panel). Therefore, RCPs have demonstrated potential not only as SWNT dispersing agents but also as versatile nanoscaled carriers to deliver a wide variety of materials into cells including targeting, therapeutic and diagnostic molecules.

### The Interaction of RCPs and SWNTs at the Molecular Level Using Computer Modeling

Experimental techniques are unable to provide a molecular level picture of the RCP/SWNT dynamic interactions, which are crucial to both dispersion strategies and practical applications. Thus, our focus has been to gain a fundamental understanding of such interactions by the use of computer simulations. Motivated by the results of our previous work on RCP/SWNT systems,<sup>14</sup> which quantified the favorable binding energy of RCPs to SWNTs, this study utilizes molecular dynamics (MD) modeling to further enhance the SWNT dispersion stability by considering RCP design modifications.

*“As drug carriers, SWNTs are capable of delivering high doses of drugs to specific tumor targets without causing damage to healthy tissue.”*

### Proposed RCP Design Modifications

Because the RCP structure plays a critical role in forming stable SWNT dispersions, we propose structural modifications to the original RCP design to explore whether an even better structure exists. Our modification involves incorporation of *m*-aminobenzoic acid (MABA), which is a benzene derivative that can form a particularly favorable interaction with the SWNT through the so-called

+ Van der Waals interaction: a weak interaction between any two molecules comprising an attractive component due to the interaction of the fluctuating dipoles on the two molecules and a repulsive component at short range to prevent the overlap of the molecules

\* Chirality: a geometric feature of an object; a chiral object lacks an internal plane of symmetry and cannot be superimposed with its mirror image. For example, hands are chiral objects which lead to the alternative term “handedness”. Amino acids are chiral (except for glycine) and the mirror images are designated the L- and D- forms. All naturally occurring amino acids in proteins are in the L- form.

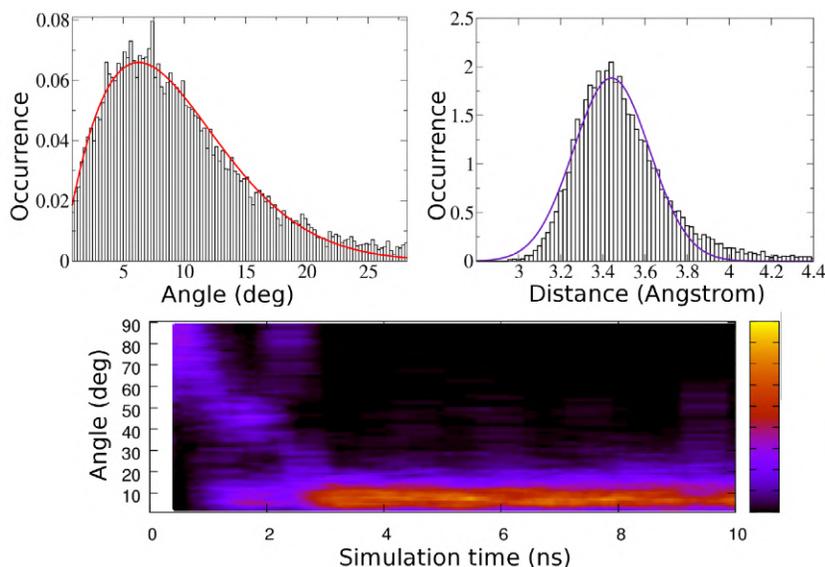


Figure 3. Plot of the  $\theta$ -angle distribution as a function of time starting from a linear configuration of Peptide-3 whose MABA rings were not initially in vdW contact with the SWNT surface. The y-axis shows the angle  $\theta$  and the x-axis gives the time for which the simulation has run. The color gradient shows the occurrence, in which yellow indicates the highest. The plot shows that fluctuations in the angle diminish when the MABA rings  $\pi$ - $\pi$  stack with the surface of the nanotube at  $\sim 2.5$  ns. Normalized distribution of the angle  $\theta$  (top left panel) and distance  $d$  (top right panel) for Peptide-3.

$\pi$ - $\pi$  stacking effect (an attractive nonbonded interaction due to the delocalization of  $\pi$ -electrons that occurs between aromatic rings oriented parallel to each other). The RCP molecule we consider here (called RC7-Cys following Dieckmann's notation) contains 17 amino acids, and each MABA substitution replaces one amino acid. The four MABA derivatives chosen for our study are comprised of one single (Peptide-1) and three double substitutions (Peptide-2, 3 and 4).

We attempt to correlate the RCP/SWNT binding affinity with the number and placement of MABA units. The two simplest possible arrangements of RCPs that encase, and hence solubilize an SWNT, are shown in Figure 1 (left panel). We suggest that the actual peptide coating on the SWNT is comprised at least partially of these arrangements. In both of these cases, hydrogen bonding between amino acids facilitates the formation of an outer-peptide cylinder shielding the SWNT (itself a carbon cylinder) from water.

Peptide-1 and 3 were previously synthesized by Dieckmann et al.<sup>15</sup> and showed significant changes in SWNT dispersibility compared to the original RCP molecule. It was hypothesized that these MABA derivatives would greatly enhance the stability of the RCP/SWNT interactions and thus would result in better SWNT dispersions, with the doubly substituted RCP being the best dispersant. However, Peptide-1 with one MABA was observed

to increase the concentration of dispersed SWNTs whereas Peptide-3 with two MABAs was observed to decrease the concentration of dispersed SWNTs (Figure 2, experimental data). These puzzling results encouraged us to investigate the detailed molecular interactions of these modified peptides with SWNTs.

### The Molecular Dynamics Method

In this study, we performed fully atomistic MD simulations on all of the systems. This is a computational method which numerically applies Newton's laws of motion to simulate the behavior of all the atoms (including solvent atoms) in a complex molecular system. The output of a simulation is the trajectories of all the atoms evolving in time, which we can visualize as a movie and analyze.

Each system is composed of one SWNT (diameter 8.7 Angstroms) and one or more of a single type of the MABA derivatives in a simulation box filled with water. More details on the simulation settings can be found in previous work carried out in the Nielsen Lab.<sup>16</sup> For each system, the SWNT/RCP interaction was characterized both in terms of energetics (thermodynamics) and dynamics (kinetics).

### Our Findings and Proposed Methodology for the Thermodynamics Study

We studied the thermodynamics of the RCP/SWNT interaction by first characterizing the binding af-

finity of the MABA units to the carbon nanotubes. We calculated the angle and distance between the SWNT surface and the plane of the MABA ring throughout the course of the MD simulations. As defined in Figure 4 (right panel), an angle of zero indicates that the MABA ring is oriented parallel to the SWNT surface, which is the optimal orientation for  $\pi$ - $\pi$  stacking. In a simulation in which the MABA rings of Peptide-2 were not initially close to the nanotube, we observed that as the peptide absorbed onto the SWNT, the MABA rings oriented themselves parallel to the SWNT surface and thereafter remained in a parallel orientation. An average angle of  $\sim 6^\circ$  and distance of  $\sim 3.5$  Angstroms from a MABA unit to the SWNT surface was consistently observed for all the MABA derivatives we studied (Figure 3), indicative of a strong  $\pi$ - $\pi$  stacking interaction between the MABA ring and the SWNT surface. It is important to note that because of the honeycomb-like structure of the SWNT surface (Figure 4, left panel), a MABA ring can form  $\pi$ - $\pi$  stacking interactions anywhere on the SWNT surface and therefore is able to “slide” along the SWNT instead of being bound to a particular location.

To further characterize the MABA/SWNT interactions, we investigated their vdW interaction energy. The MABA/SWNT vdW energy is defined as the sum of the vdW energy over all pairs of atoms  $i$  and  $j$  with atom  $i$  in the MABA molecule and atom  $j$  in the SWNT molecule:

$$U(r) = \sum_{i,j} \epsilon_{ij} \left[ \left( \frac{R_{min_{ij}}}{r_{ij}} \right)^{12} - 2 \left( \frac{R_{min_{ij}}}{r_{ij}} \right)^6 \right]$$

where  $\epsilon_{ij}$  is the energy minimum,  $r_{ij}$  is the distance between the two atoms, and  $R_{min_{ij}}$  indicates the distance at which the vdW energy is zero.

For each vdW energy calculation, we ran a preliminary simulation to allow the system to equilibrate before we collected data. A comparison of the vdW energy of only the SWNT-bound MABA ring segment among the different MABA derivatives, with the disulfide bond formed or broken, all yielded similar values (data not shown). This, combined with the angle and distance data, confirmed

that: (1) The SWNT-binding affinity of the MABA ring portion of the RCP molecules in systems with the same number of MABA substitutions is similar, and (2) the affinity between peptides and SWNTs increases with increasing MABA substitution. From this evidence, we hypothesized that the MABA units themselves are not directly responsible for differences in the SWNT/RCP interactions. Rather, the presence of MABA units in different positions causes conformational differences in how the peptides wrap around and hence bind to carbon nanotubes.

The MD simulations also allow us to visualize the absorption process of RCPs onto the SWNT, which, combined with what is known from the

experimental data, can be broken into several steps: (1) Peptides in aqueous solution approach a SWNT. (2) The pep-

tides initially absorb onto the SWNT surface with random conformations where the MABA units play an important role in maintaining contact between the SWNT and RCPs. (3) Sonication (a procedure in which ultrasound is utilized to agitate the system and fray the ends of carbon nanotube bundles so that the RCPs can insert in between the SWNTs and separate them into individual nanotubes) adds a significant amount of energy to the system, giving the peptides greater freedom to sample conformations that enhance their interaction with the SWNT and with each other. (4) Sonication also promotes disulfide bond formation (because air bubbles created by sonication contain oxygen, which chemically oxidizes the cysteine amino acids to create a disulfide bond) between adjacent terminal cysteine amino acids, either on the same or on different peptides, to create cyclized or polymerized peptides, respectively.

The overall result of this process is the formation of macromolecular arrangements of peptides, which effectively protect the SWNT surface from water. From our simulations of the double-substituted peptides, we saw that the farther apart the MABA units are spaced in the RCP molecule, the more difficult it is for the peptide to find a good SWNT-binding conformation, especially when the initial MABA/SWNT  $\pi$ - $\pi$  stacking causes the middle portion of the peptide to buckle and make poor

*“The output of a simulation is the trajectories of all the atoms evolving in time, which we can visualize as a movie and analyze.”*

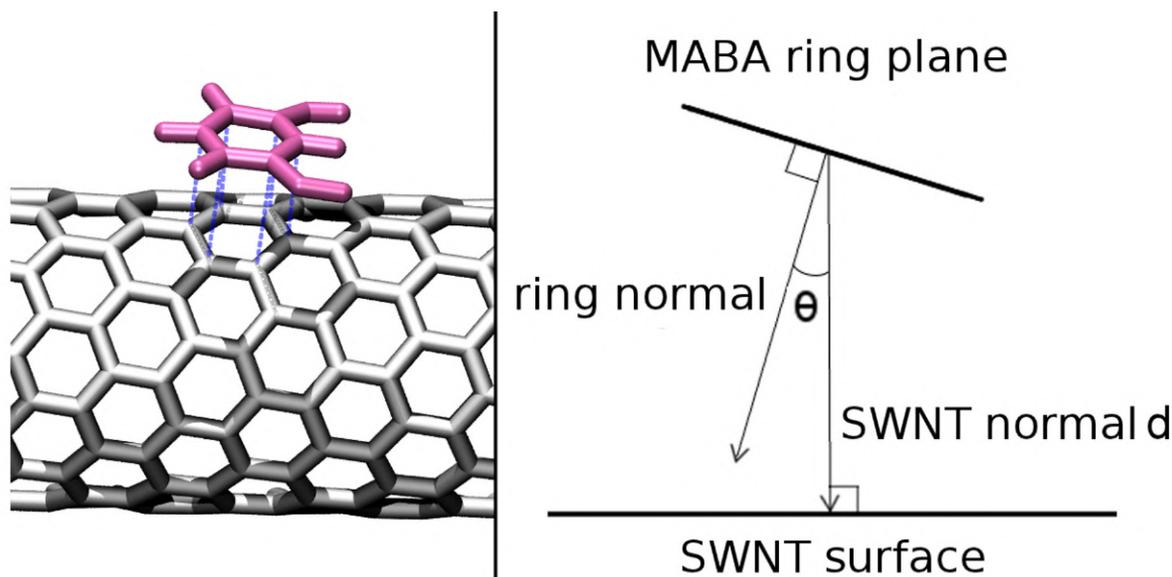


Figure 4.  $\pi$ - $\pi$  stacking interaction between a MABA ring and a SWNT surface. Schematic to define the angle and distance between the MABA ring and the SWNT surface (right). The angle  $\theta$  is made by the normal of the SWNT long axis and the normal of the MABA plane. The distance  $d$  is the length of SWNT normal vector whose tail ends at the center of mass of the ring. The most favorable energy for  $\pi$ - $\pi$  stacking is for  $\theta = 0$ .

contact with the SWNT. We thus suggested that Peptide-1 and Peptide-2 have some advantages over the other RCP substitutions because the MABA(s) in the middle of the molecule improve the binding affinity with the SWNT, yet allow the two “arms” to tightly wrap the nanotube. To test this idea, we calculated the SWNT-binding vdW energies of all the MABA derivatives. We hypothesized that the farther the MABA units were spaced on the peptide, the more unfavorable the vdW energy would be. Our data showed the three double substitution systems yielded significantly different vdW energies. Moreover, by considering RCP wrapping with or without disulfide bond formation, the relative vdW energies were also notably different. For systems in which the peptide is cyclized around a SWNT, Peptide-2 had the most favorable vdW energy and Peptide-4 the least favorable, which supported our hypothesis. Interestingly, for systems in which the peptide is wrapped but not cyclized around a SWNT, Peptide-3 had a more favorable vdW energy than Peptide-2, despite its two MABA units being farther apart. This result warrants further study.

One direction of further study is to explore the possibility that the puzzling result discussed above is due to an inadequate exploration of peptide conformations. Specifically, since the MD simulations do not account for the additional energy provided to the system due to sonication, the ability of the peptides to explore conformations that would bind

well to an SWNT is limited. We plan to utilize the replica exchange technique in order to overcome this possible conformational sampling problem. The underlying principle of this method is based on the fact that at higher temperatures, atoms in a system have a higher kinetic energy (and accordingly move faster), and this increased energy increases the conformational freedom of the molecules. Replica exchange involves heating and cooling the system periodically to enhance its ability to access new conformations.

### Proposed Methodology for Kinetics Study

While thermodynamics is concerned with how energetically favorable one SWNT-bound RCP conformation is compared with another, kinetics is concerned with how quickly an RCP molecule can switch between different conformations. On the molecular scale, there are many ways one could characterize the kinetics of the RCP/SWNT association. One way would be to ask how quickly a peptide would wrap around and bind to a SWNT if it approached from the aqueous solution. We could characterize wrapping by an energetic criterion, namely when the RCP/SWNT vdW energy exceeds some threshold value. This criterion is independent of any particular conformation of the SWNT-binding peptides. The initial peptide conformation consistent with “approaching from the aqueous solution” could be chosen as follows: We could per-

form an MD simulation of a linear peptide inside a spherical cage slightly larger than the length of the extended peptide and located just beyond vdW interaction range of the SWNT. In this manner, the peptide would be allowed to sample different conformations within its cage in order to mimic realistic conformations of peptides coming from the aqueous solution. The peptide would then be given an initial velocity  $v_0$  in order to guide it towards the nanotube. The peptide that takes the least amount of time to wrap the SWNT (by exceeding the chosen vdW energy threshold) would have the most kinetically favorable binding to the nanotube.

### Conclusions and Future Directions

In this study, we proposed structural modifications of the RCP molecule involving incorporation of MABA units in order to improve its SWNT dispersing ability. Some of these modified peptides have been shown in experiments to notably change SWNT solubility. We utilized MD computer simulations to understand these differences in terms of the molecular-level RCP/SWNT interactions. We found that the RCP/SWNT vdW energies were different among the different MABA derivatives. We also observed a correlation between the number and placement of MABA rings and the RCP/SWNT binding affinity. Further studies as outlined in this paper ultimately would enable us to gain molecular insight into which peptide design modifications lead to more effective SWNT dispersions.

### Acknowledgments

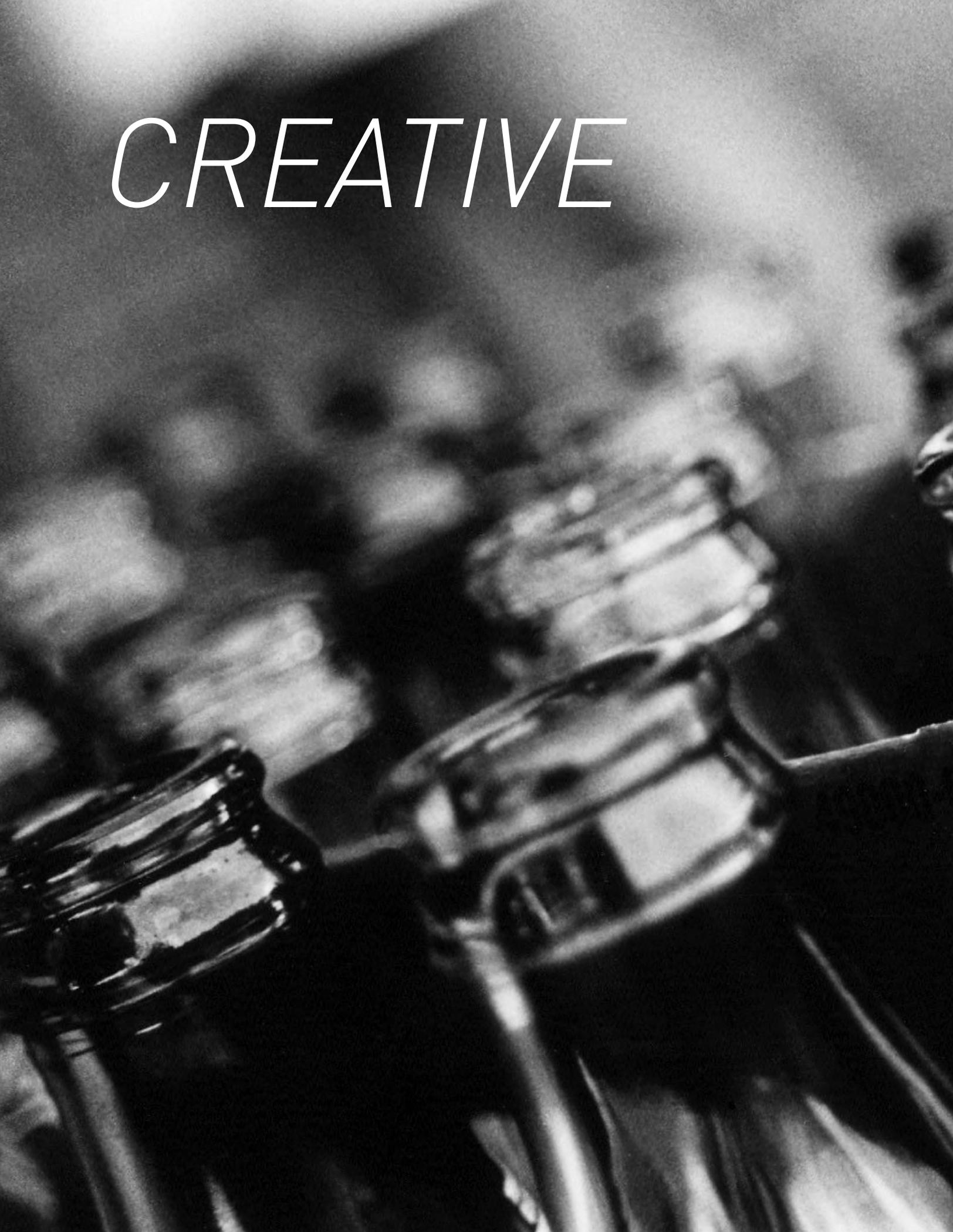
The RCP systems were designed and synthesized by Dr. Gregg Dieckmann and his lab team. In particular, Dr. Dieckmann's graduate student, Anton Klimenko, contributed significant insight and experimental data that made this study possible. I owe all my skills, knowledge, and passion for computational chemistry to Dr. Steven Nielsen and graduate student Udayana Ranatunga of the Nielsen lab.

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*CREATIVE*





6

2 OZ. BOTTLES

# Nostalgia

*by Linda Wilson*



Black and white photography is fascinating to me, because it is based on simple elements. The challenge for the photographer is to forget about colors and transform that simplicity to bring out an object's form, using only tone and light. Without the distraction of color, the photograph can then be appreciated for its graphic elements and composition.

The subjects in these photographs (page 64-65 and adjacent) are everyday items which evoke feelings of nostalgia. Soda pop bottles become lazy summer afternoons at the country store. Hand tools are transformed into memories of Dad working in his shop. Graphic qualities of light, shapes, and patterns turn functional items into dreamlike visions of days gone by.

# Wooden Canyon

*by Micheal Ansley*



I find beauty in the smallest details of objects and things found in everyday life that may be missed by many due to the rushed pace that is modern life. When I take a photograph, it usually is of something that most people have encountered but might not have had the time to consider its hidden beauty, story, and wisdom. I hope my photographs serve as a reminder to those who see them to slow down enough occasionally to consider their world from a different perspective. For instance, the subject of the Wooden Canyon is probably something that most wouldn't even give a second glance to, while passing it every day in between the parking lot and the door of their building.

Simply looking closer at it reveals much about what the tree once was, will be and is presently. Most would see it as just a dead stump, but I see it as a representation of limbo. It could have once been a shade tree, living for many years according to its rings. Now it is but a representation of human development, a placeholder for what is to replace it. Limbo is the in-between, the gray on the color scale of life; this is why I felt it best expressed as a black and white photograph. The "Canyon" in the photograph is a glimpse into the abyss that the stump will eventually meet.

# Home

by *Brittany Sharkey Andrews*

Urban lights bathe alien colours across lifeless snowed decor  
 And lonely breezes drop a gentle white lace on empty tree limbs,  
 Reminiscent of the delicate white sheets quietly cloaking the humble  
 nude left to her soft mounds of pillows [to fill the space you once did].  
 Coffee, humid heating vents, and something sautéed linger on the air  
 from morning to last call

When the image of you saunters home to the lowing sounds of bus  
 brakes and gear shifts, sharp barks of territorial dogs kept at distance,  
 and fragmented voices that pick up like paper in the wind.

Yet the stiff firs, for all their green, don't rustle like the leafy pecans on  
 a mild March night

And empty bottles rolling along the pavement don't quite sing like the  
 chimes on the porch in a lazy spring Sunday's soft breeze.

Dismiss the thoughts with the taste of vodka still on the back of your  
 tongue, tighten the coat,

and convince there's something redeeming in all this used and  
 [crowded] barren space.

But, if you pause for a moment in the warmth leaking from that door,  
 take a second before re-entering that stage... close your eyes and  
 breathe...

- Oh, can't you hear it?

Like a long lost first love, the land is calling you back to her,

Promising scents of spring throughout the year

And batting lashes of long grass fields.

Her body rolls, dips, and sighs with the wind,

Hugging the sweet sunlight like a summer dress

On the woman's thighs that someday your children will cling to -

Perfumed in the morning by dew and fresh budded grass, and in the  
 dusk by home-cooked meals and the setting sun's kisses breathing on  
 the earth.

She's traditional, but fresh, all at once

And chatty in the pattern of birdsong and laughter -

A little less interesting than the northern city's many facades

But her faith in earnest runs as deep as the dirt

Turned over by many rough hands and reshaped by those that tried to  
 love her before.

Here is a home you knew first.  
 And here is the home that will hold steadfast and patient  
 Until your explorations of the world reach a point of self-satisfaction.  
 While you scale sky scrapers and networking ladders  
 And snack on delicate pastries and fine wines mimicking exotic  
 pleasures,  
 This is the home that will be home when you're ready to tell the stories  
 of how you've seen it all  
 And done the unthinkable:  
 Traveled Europe by the map of your stomach  
 Took a dive in foreign waters bluer than your eyes  
 Or stood face to face with Lincoln and Jefferson in the same day  
 To small ears perched on your lap and at your feet  
 Dying to get out and test their own restless ambitions.  
 And all the meanwhile, this home will patiently keep your secret and  
 her pride  
 Quiet and slow to reveal that there's no place quite like the home of a  
 cool October breeze that plays on still green leaves;  
 of the hot August night that persuades work to wait another day;  
 of the soft green grass of February that welcomes barefoot walks  
 where a week before there was snow and ice;  
 and absolutely no place like the home of the love and two arms made  
 especially just for you, all year round.  
 The world offers your spirit adventure, ensnares your mind's  
 imagination with stories untold,  
 and, heaven help you, may those wonders never lose their  
 enchantment.  
 But, lest you ever come close, don't ever forget:  
 this home will always hold your heart.  
 [And she waits for you]

*Music is a highly expressive form and success in finding a melody that matches emotion is not difficult. However, in those moments that other people's music falls short, I turn to my own form. In the traditional music sense, I have little to no musical talent beyond reading music and the Bb clarinet. My form is verbal music: poetry. Although I never adhere to a true pattern of meter or rhyme, the beauty of the unconstrained natural rhythm of language never fails to captivate me and I attempt to draw this beauty into my own use of the tongue. True to this philosophy, I don't take extremes to find obscure words or to fit my sentences to a specific syllabic quota. Casual vernacular presented with a few thoughtful twists, like a photo taken of something simple at just the right angle, can be very effective in letting people come that much closer to understanding the emotion behind my poetry.*

# Hungry Octopus

*by Rebecca Aguilar*

After making hundreds of sketches of people for a figure drawing class, it was time to show off those new skills in one big final drawing. Our ideas were only limited by the size of the paper and the messiness of the charcoal. Since I frequently go through multiple ideas, I decided to sketch out some thoughts before settling on something I liked. Initially, I thought about drawing a human figure while emphasizing the muscles to demonstrate how the human figure is like a structure. Yet, the idea felt too stereotypical, and uncreative. I wanted to do something challenging and unique.

Suddenly, an idea popped into my head quite unexpectedly, as most ideas do. Why not an octopus? A huge scary one? I had never drawn an octopus before (aside from a simple cartoony one). Taking it a step further, I decided to experiment with foreshortening (extreme perspective) by choosing a different view angle. This provided another challenge for me, as I struggle with drawing things from extreme angles, let alone an octopus. I decided to go with an interesting composition in which a gargantuan octopus menaces an unfortunate, disoriented person. To complete the weirdness, I decided to add contrasting shadows and bright lights (contrast always makes something look outstanding). Prior to beginning the drawing, I did several sketches of octopi to ensure that

my octopus looked believable. At the time, my drawing style was heavily influenced by *Invader Zim*, a television show which I had recently discovered on Nickelodeon. One will find characteristic *Invader Zim* windows and lighting throughout the composition. My drawing also contained elements characteristic of comic book panels: extreme angle, high contrast, and strange juxtapositions. I worked on the drawing in multiple spurts per day throughout the week. However, as I began reaching the endpoint of the drawing process, I suddenly began to fall ill with a cold. Soon, the drawing became a personal metaphor for how my body would hopefully fight off the horrible pathogens that were making me feel miserable.

My classmates found the drawing humorous and charming. As I've discovered, I tend to juxtapose seemingly unrelated objects, giving them a ridiculousness that draws the viewer into the drawing. Through this drawing I challenged myself and strengthened my ability at drawing octopi, lights, and extreme perspectives. I also gained a beautiful drawing that I could admire and enjoy. As for the cold, it soon went away. I think it was the octopus.

As a final note: this drawing was our final for ARTS 3367 Figure Drawing taught by Greg Metz.



