## AN HONORS UNIVERSITY IN MARYLAND











# 18th Annual Summer Undergraduate Research

Fest

Hosted by the College of Natural and Mathematical Sciences

### Wednesday, August 5, 2015 University Center, Ballroom Third Floor

#### Sponsors of the Participants in the 2015 Summer Undergraduate Research Fest: DREU Distributed Research Experiences for Undergraduates **HHMI Scholars** Howard Hughes Medical Institute HPC REU Interdisciplinary Program in High Performance Computing-A National Science Foundation's Research Experiences for Undergraduates Site **JCET** Joint Center for Earth Systems Technology-Earth Science Explorers Program MARC U\*STAR Minority Access to Research Careers-Undergraduate Student Training in Academic Research Program-NIH/National Institute of General Medical Sciences SBTP Summer Biomedical Training Program - CNMS and the UMBC Graduate School UBM Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences-National Science Foundation



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DREU	Distributed Research Experiences for Undergraduates
HHMI Scholars	Howard Hughes Medical Institute
HPC REU	Interdisciplinary Program in High Performance Computing—A National Science Foundation's Research Experiences for Undergraduates Site
JCET	Joint Center for Earth Systems Technology—Earth Science Explorers Program
MARC U*STAR	Minority Access to Research Careers —Undergraduate Student Training in Academic Research Program—NIH/National Institute of General Medical Sciences
NSA Scholar	National Security Agency Scholar
SBTP	Summer Biomedical Training Program — CNMS and the UMBC Graduate School
UBM	Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences—National Science Foundation

## **Event Schedule**

### Wednesday, August 5, 2015

All events will be held in the Ballroom, University Center, 3rd Floor

### 8:30 am: Poster Set-up & Presenter Check-In Begins

Ballroom Lobby, University Center, 3rd Floor Light Breakfast served

### 9:00 am - 10:30 am: Introductions & Oral Presentations

Ballroom, University Center, 3rd Floor

Hannah Carter & Aishwarya Iyer	Independent Research
Casey Means	DREU
Amit Nayak & George Jeffreys	HPC REU
Mario Rodriguez	SBTP
Eric Valenzuela & Alec Beri	HPC REU

### 10:30 am - 12:00 noon: Poster Presentations

Ballroom, University Center, 3rd Floor

10:30 am – 11:15 am – Poster Session 1 11:15 am – 12:00 noon – Poster Session 2

### 12:00 noon – 12:30 pm: Mentor Recognition and Closing

Ballroom, University Center, 3rd Floor

## Welcome

Welcome to the eighteenth annual UMBC Summer Undergraduate Research Fest, which is hosted by the College of Natural and Mathematical Sciences. It is inspiring to see so many students from near and far presenting the results of their summer research projects. Some of these projects are the result of independent agreements, but most have been made possible by grants or other funding dedicated to encouraging undergraduate research. All projects are tied in some way to UMBC and require the support of research mentors, whose passion for science and commitment to education are truly exceptional. I commend the students on their extraordinary efforts this summer, and thank each of the faculty, staff and graduate student mentors who have worked so closely with them. Especially, I want to thank Kathy Sutphin, the Assistant Dean for Academic Affairs, who coordinated this special occasion with Justine Johnson. Associate Director of the Meyerhoff Graduate Fellows Program, and Andrea Miller, STEM Program Coordinator. Best wishes for a very successful event.

William R. LaCourse, Ph.D.Dean and ProfessorCollege of Natural and Mathematical Sciences

## SURF's 2015 Outstanding Mentors

At this 18th Annual Summer Undergraduate Research Fest, we are pleased to acknowledge all of the researchers who have supported student researchers in their laboratories as "Outstanding Mentors" for 2015

A research mentor is a trusted guide who supports and facilitates a mentee's development towards the realization of his or her short and long-term career and life goals. A research mentor also educates and encourages young scientists about the opportunities available to them as they consider careers in research. A research mentor also provides precious access to his or her research laboratory or project and gives mentees opportunities to contribute toward the 'active' scientific research activities, which may not otherwise be available to high school or undergraduate students.

On behalf of the College of Natural and Mathematical Sciences, the Program Directors and Coordinators of the UMBC Summer Research Programs, and especially the many participants in this summer's guided research experiences, we thank these mentors for their ongoing support of student research and for their willingness to invest their time and resources to contribute to UMBC's rich history of undergraduate research support. We would also like to give special thanks to all of the post docs, graduate students and undergraduates in their research groups who have worked so diligently to support the mentoring of these SURF participants.

It is with sincere appreciation that we honor the following researchers as the 2015 Outstanding Mentors of the 18th Annual CNMS Summer Undergraduate Research Fest:

Mentor Name	Presenter Name	Affiliation
Dr. Kofi Adragni	Trevor Adriaanse	HPC REU
	Ely Biggse	HPC REU
	Tessa Helble	HPC REU
	Meshach Hopkins	HPC REU
	George Jeffreys	HPC REU
	Amit Nayak	HPC REU
	Rebecca Rachan	HPC REU
	Subodh Selukar	HPC REU
Dr. Charles Bieberich	Haneet Chadha	MARC U*STAR Trainee
	Megha Kori	Independent Research
		Independent Research
Dr. Lee Blaney	Hollie Adejumo	Independent Research
	Graham Rubin	Independent Research

Mentor Name	Presenter Name	Affiliation
Dr. Stacy Branham	Imani McLaurin	DREU
Dr. Rachel Brewster	Caitlin Ford	Indepentdent Research
	Eudorah Vital	HHMI Scholar
	Jonathan Werner	Independent Research
Dr. Joseph Bryant	Lauryn Mitchell	HHMI Scholar
Dr. Mauricio Bustos	Tiana Boardley	MARC U*STAR Trainee
Dr. Ruben Delgado	Julio Roman	JCET
	Shelbi Tippett	JCET
Dr. Belay Demoz	Glorianne Rivera-	JCET
	Christian Sias	JCET
Dr. Chris Geddes	Greg Brinsley	Independent Research
	Jacob Dohl	Independent Research
	Karen Losito	Independent Research
	Maraki Negesse	Independent Research
Dr. Matthias Gobbert	Fernando Avila-Soto	HPC REU
	Alec Beri	HPC REU
	Wesley Collins	HPC REU
	Changling Huang	HPC REU
	Christopher Lowman	HPC REU
	Daniel Martinez	HPC REU
	Michael Monaghan	HPC REU
	Alexey Munishkin	HPC REU
	Brandon Osborne	HPC REU
	Gabrielle Salib	HPC REU
	Eric Valenzuela	HPC REU
	Abenezer Wudenhe	HPC REU
Dr. Erin Green	Grace Choi	UBM
	Oluwagbotemi Igbaroola	MARC U*STAR Trainee
	Rushmie Kulkarni	UBM
Dr. Christopher Hennigan	Adrian Davey	HHMI Scholar
	Travis McKay	HHMI Scholar
Dr. Kathleen Hoffman	Adam Byerly	UBM
Dr. Amy Hurst	Chuk Amaefule	Independent Research
	Braxton Dubin	Independent Research
	Casey Means	DREU
	Lisa Nguyen	Independent Research
		MARC U*STAR Trainee
Dr. Anthony Johnson	Elangeni Yabba	SBTP Trainee
Dr. Jacob Kogan	Alvaro Arrospide Fletcher	MARC U*STAR Trainee

Mentor Name	Presenter Name	Affiliation
Dr. Minjoung Kyoung	Sarah Pollock	MARC U*STAR Trainee
Dr. William LaCourse	Malique Georges	SBTP Trainee
	Charles Gray	SBTP Trainee
	Chloe Kwon	Independent Research
Dr. Jennie Leach	Alicia Khan	MARC U*STAR Trainee
Dr. Weihong LIn	Mario Rodriguez	SBTP Trainee
	Chantel Wilson	HHMI Scholar
Dr. Lasse Lindahl	Rebekah Rashford	HHMI Scholar
Dr. Bernard Lohr	Julia Gao	Independent Research
Dr. Mark Marten	Pranesh Navarathna	Independent Research
Dr. Helena Mentis	Veeha Khanna	DREU
	Monica Martinez	DREU
Dr. Stephen Miller	Courtney Bass	Independent Research
	Binika Chunara	Independent Research
	Jordan Damon	Independent Research
	Beatrice Rukenwa	Independent Research
	Rima Sakhawala	MARC U*STAR Trainee
Dr. Christopher Murphy	Ana Maldonado	SBTP Trainee
Dr. Nagaraj Neerchal	Joseph Emelike	HPC REU
	David Harper	HPC REU
	Charlotte Mann	HPC REU
	Kwame Owusu-Boaitey	HPC REU
Dr. Suzanne Ostrand-Rosenberg	Ramses Long	Independent Research
Dr. Bradford E. Peercy	Amanda Alexander	HPC REU
	Erin DeNardo	HPC REU
	George Eskandar	HPC REU
	Eric Frazier	HPC REU
	Samantha Furman	MARC U*STAR Trainee
	Jennifer Houser	HPC REU
	Samuel Keating	Independent Research
	Michael McCauley	HPC REU
	Lindsay Mercer	UBM
	Ellen Prochaska	HPC REU
	Nicholas Rojina	HPC REU
	Jessica Wojtkiewicz	HPC REU
Dr. Marcin Ptaszek	Melissa Lucero	MARC U*STAR Trainee
Dr. Phyllis Robinson	Tahsin Khan	UBM

Mentor Name	Presenter Name	Affiliation
Dr. Michelle Starz-Gaiano	Lilian Anosike	UBM
	Margarita Brovkina	Independent Research
	Kamsi Odinammadu	MARC U*STAR Trainee
	Amelia Smith	Independent Research
Dr. Michael Summers	Alecia Achimovich	SBTP Trainee
	Tawakalitou Alabi	SBTP Trainee
	Tiffany Bamfo	SBTP Trainee
	Andrew Brown	SBTP Trainee
	Grace Canham	SBTP Trainee
	Paige Canova	Independent Research
	Hannah Carter	Independent Research
	Eric Cormack	SBTP Trainee
	Emily Diaz	Independent Research
	Geraldine Ezeka	Independent Research
	Heather Frank	Independent Research
	Shyohn Ghorbanpoor	SBTP Trainee
	Lindsay Glang	Independent Research
	Tarik Hawkins	MARC U*STAR Trainee
	Aishwarya Iyer	Independent Research
	Mian Khalid	Independent Research
	Michael Lopresti	Independent Research
	1	MARC U*STAR Trainee
	Briaunna Minor	SBTP Trainee
	Chang-Wu Mungai	SBTP Trainee
	Colin O'Hern	Independent Research
	DianneMarie Omire-	
	Mayor	SBTP Trainee
	Amalia Rivera-Oven	Independent Research
		HHMI Scholar
		MARC U*STAR Trainee
	Justin Santos	SBTP Trainee
	Carly Sciandra	Independent Research
	Zoe Spadaro	SBTP Trainee
	Roald Teuben	Independent Research
	Kechera Tilghman	SBTP Trainee
	Ae Lim (Ally) Yang	Independent Research
	Jessica Zaki	Independent Research
Dr. Cynthia Wagner	Natithorn Bhusri	Independent Research
	Alex Kuznetsov	Independent Research

### **Alphabetical Listing of Poster Presenters**

First Name	Last Name	Poster	Poster #
		Session	
Alecia	Achimovich	Session 1	31*
Hollie	Adejumo	Session 2	88
Trevor	Adriaanse	Session 1	51*
Tawakalitou	Alabi	Session 1	57*
Amanda	Alexander	Session 2	16*
Chuk	Amaefule	Session 2	64
Lilian	Anosike	Session 1	75*
Alvaro	Arrospide Fletcher	Session 1	13
Fernando	Avila-Soto	Session 1	27*
Tiffany	Bamfo	Session 1	43*
Courtney	Bass	Session 1	73
Natithorn	Bhusri	Session 1	37*
Ely	Biggse	Session 2	8*
Tiana	Boardley	Session 2	24
Greg	Brinsley	Session 1	49
Margarita	Brovkina	Session 2	50
Andrew	Brown	Session 1	81*
Adam	Byerly	Session 1	69*
Grace	Canham	Session 2	82*
Paige	Canova	Session 2	56*
Haneet	Chadha	Session 2	46
Grace	Choi	Session 1	3*
Binika	Chunara	Session 1	95
Wesley	Collins	Session 2	22*
Eric	Cormack	Session 1	21
Jordan	Damon	Session 2	100
Adrian	Davey	Session 1	5
Erin	DeNardo	Session 1	15*
Emily	Diaz	Session 1	65*
Jacob	Dohl	Session 1	89*
Braxton	Dubin	Session 2	72
Joseph	Emelike	Session 2	86*
George	Eskandar	Session 1	79*
Geraldine	Ezeka	Session 1	61*
Caitlin	Ford	Session 1	83
Heather	Frank	Session 2	102*
Eric	Frazier	Session 2	16 *

\* Indicates research that is co-presented, half of the group is assigned to present during session 1 and the other half is assigned to present during session 2.

### Alphabetical Listing of Poster Presenters (continued)

First Name	Last Name	Poster	Poster #
		Session	
Samantha	Furman	Session 1	39
Julia	Gao	Session 1	1
Malique	Georges	Session 2	60
Shyohn	Ghorbanpoor	Session 1	87
Lindsay	Glang	Session 1	23
Charles	Gray	Session 2	42
David	Harper	Session 1	85*
Tarik	Hawkins	Session 2	32*
Tessa	Helble	Session 1	7*
Meshach	Hopkins	Session 2	52*
Jennifer	Houser	Session 2	80*
Changling	Huang	Session 1	47*
Oluwagbotemi	Igbaroola	Session 2	92
Samuel	Keating	Session 2	2
Mian	Khalid	Session 2	94*
Alicia	Khan	Session 1	53
Tahsin	Khan	Session 2	70*
Veeha	Khanna	Session 1	35
Megha	Kori	Session 2	68
Rushmie	Kulkarni	Session 2	4*
Alex	Kuznetsov	Session 2	38*
Chloe	Kwon	Session 1	77
Ramses	Long	Session 1	99
Michael	Lopresti	Session 1	63
Karen	Losito	Session 1	59
Christopher	Lowman	Session 1	47*
Melissa	Lucero	Session 1	67
Ana	Maldonado	Session 1	25
Charlotte	Mann	Session 1	85*
Monica	Martinez	Session 1	29
Daniel	Martinez	Session 2	18*
Michael	McCauley	Session 2	16*
Travis	McKay	Session 2	20
Imani	McLaurin	Session 1	91
Lindsay	Mercer	Session 2	76*
Briaunna	Minor	Session 1	101*
Lauryn	Mitchell	Session 2	78
Michael	Monaghan	Session 1	17*

\* Indicates research that is co-presented, half of the group is assigned to present during session 1 and the other half is assigned to present during session 2.

### Alphabetical Listing of Poster Presenters (continued)

First Name	Last Name	Poster	Poster #
		Session	
Chang-Wu	Mungai	Session 2	66*
Alexey	Munishkin	Session 1	17*
Pranesh	Navarathna	Session 2	74
Maraki	Negesse	Session 2	90*
Lisa	Nguyen	Session 1	71
Kamsi	Odinammadu	Session 1	9
Colin	O'Hern	Session 1	55*
DianneMarie	Omire-Mayor	Session 1	93*
Brandon	Osborne	Session 2	48*
Kwame	Owusu-Boaitey	Session 2	86*
Sarah	Pollock	Session 2	10
Ellen	Prochaska	Session 2	80*
Rebecca	Rachan	Session 2	52*
Rebekah	Rashford	Session 2	6
Amalia	Rivera-Oven	Session 2	58*
Glorianne	Rivera-Santiago	Session 2	40
Nicholas	Rojina	Session 1	15*
Julio	Roman	Session 2	34*
Graham	Rubin	Session 2	36
Beatrice	Rukenwa	Session 2	96
Rima	Sakhawala	Session 1	19
Gabrielle	Salib	Session 2	48*
Justin	Santos	Session 2	98*
Carly	Sciandra	Session 1	97*
Subodh	Selukar	Session 1	51*
Christian	Sias	Session 2	84
Amelia	Smith	Session 2	54
Zoe	Spadaro	Session 1	57*
Roald	Teuben	Session 2	62*
Kechera	Tilghman	Session 2	44*
Shelbi	Tippett	Session 1	33*
Eudorah	Vital	Session 1	11*
Jonathan	Werner	Session 2	12*
Chantel	Wilson	Session 2	30
Jessica	Wojtkiewicz	Session 1	79*
Abenezer	Wudenhe	Session 2	28*
Elangeni	Yabba	Session 2	26
Ae Lim (Ally)	Yang	Session 1	41
Jessica	Zaki	Session 2	14

\* Indicates research that is co-presented, half of the group is assigned to present during session 1 and the other half is assigned to present during session 2.

## **Oral Presentations**

1	Hannah Carter & Aishwarya Iyer	Independent Research
2	Casey Means	DREU
3	Amit Nayak & George Jeffreys	HPC REU
4	Mario Rodriguez	SBTP
5	Eric Valenzuela	HPC REU

### **Program Acronyms**

DREU	Distributed Research Experiences for Undergraduates
HHMI Scholars	Howard Hughes Medical Institute
HPC REU	Interdisciplinary Program in High Performance Computing—A National Science Foundation's Research Experiences for Undergraduates Site
JCET	Joint Center for Earth Systems Technology—Earth Science Explorers Program
MARC U*STAR	Minority Access to Research Careers —Undergraduate Student Training in Academic Research Program—NIH/National Institute of General Medical Sciences
NSA Scholar	National Security Agency Scholar
SBTP	Summer Biomedical Training Program — CNMS and the UMBC Graduate School
UBM	Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences—National Science Foundation
UMBC	University of Maryland, Baltimore County

### DIMERIZATION STUDIES OF WILD TYPE AND TSL4 $\Delta$ PBS CONSTRUCTS OF HIV-1 5' UTR

#### Hannah Carter, Aishwarya Iyer, Joshua Brown, Michael F. Summers Department of Chemistry and Biochemistry, Howard Hughes Medical Institute, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Human Immunodeficiency Virus Type 1 (HIV-1) patients are treated with a drug cocktail that targets various points in the viral life cycle, which unfortunately comes with myriad side effects and the possibility of resistant strains due to the high mutation rate of the virus. There is no drug available, however, that targets the translation or genome recognition portion of the lifecycle, which is characterized by an equilibrium between the monomer and dimer conformations of the highly conserved 5' Leader (5'-L) in the HIV-1 RNA genome.

In order to study the structure of the monomer conformation using Nuclear Magnetic Resonance (NMR), 5'-L monomer must be isolated and reduced to its smallest functional core. The Primer Binding Site (PBS) region adds broad and crowded signals to our NMR spectrum, making the assignment of peaks difficult. We compared the construct in which the PBS region was removed to the wild type construct to determine how the PBS region affects the dimerization of the RNA. We used gel shift assays with varying incubation times and concentrations to determine this. So far, results indicate that our construct without PBS dimerizes similarly to our wild type, implying that the  $\Delta$ PBS construct can act as an analog for the wild type in further studies.

This research was funded by NIH/NIGMS grant *1P50GM103297*, and was conducted at the Howard Hughes Medical Institute at UMBC with support in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. We would also like to thank our research team Seungho Choi, Eric Cormack, and Shyohyn Ghorbanpoor for their assistance.

#### PRECISE, PREDICTIVE, PERSONALIZED: DESIGNING ASSISTIVE NOTIFICATIONS AND ADAPTATIONS FOR POINTING PERFORMANCE

<u>Casey Means</u><sup>1</sup>, Abdullah Ali<sup>2</sup>, Aqueasha Martin Hammond<sup>2</sup>, Amy Hurst<sup>2</sup> <sup>1</sup>Department of Computer Science, Rhodes College, 2000 North Parkway, Memphis, TN 38112 <sup>2</sup>Department of Information Systems, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

The Internet should be accessible to all users. However, computers are frequently illequipped to handle the unique needs of users with varying abilities. People who find it difficult to use a pointing device, like a mouse, may find it frustrating to use a computer. Many factors, such as age, physical impairment, or fatigue, can affect pointing performance and pointing device use. Adaptive user interfaces (AUIs) are spaces where people interact with computers and computer change to suit users' needs. As such, they can make computer more accessible to people that find it difficult to complete pointing tasks. However, to be useful, their design must not outweigh their convenience.

We conducted a study with 11 younger adults to test a Chrome Extension prototype. It detects pointing performance, notifies the user of any problems, and provides assistance. We asked the younger adults for feedback on our designs and to discuss what they liked and disliked. We found they preferred notification with functionality attached. They were also interested in data about their performance. As for adaptations, they preferred a hybrid system, because it provided the convenience of a computer while keeping them in control. However, they were also concerned with how precisely the computer could adapt to their needs. In addition to this study, we have designed and developed new adaptations to address cursor loss and menu slips, both common pointing problems. These have been integrated in prototype for future work. In the future we will focus on both adaptations and notifications and address potential solutions for specific pointing problems.

I would like to thank the Computing Research Association's Distributed Research Experiences for Undergraduates (CRA-DREU) program for both financial sponsorship and opportunity. I would also like to thank the University of Maryland, Baltimore County for its support. Finally, I sincerely thank Dr. Amy Hurst, Dr. Aqueasha Martin Hammond, Abdullah Ali, and everyone in the UMBC PAD Lab for their help.

### NUMERICAL EVALUATION OF MINIMUM AVERAGE DEVIANCE ESTIMATION IN ULTRA HIGH DIMENSIONAL POISSON REGRESSION

REU Site: Interdisciplinary Program in High Performance Computing <u>Ely Biggs</u><sup>1</sup>, <u>Tessa Helble</u><sup>2</sup>, <u>George Jeffreys</u><sup>3</sup>, <u>Amit Nayak</u><sup>4</sup>, Graduate assistant: Elias Al-Najjar<sup>2</sup>, Faculty mentor: Kofi P. Adragni<sup>2</sup>, Client: Andrew Raim<sup>5</sup> <sup>1</sup>Department of Applied Mathematics, Wentworth Institute of Technology <sup>2</sup>Department of Mathematics and Statistics, UMBC <sup>3</sup>Department of Mathematics, George Washington University <sup>4</sup>Department of Mathematics, George Washington University <sup>5</sup>US Census Bureau

The second most expensive part of US Census Bureau's decennial census in 2010 was Address Canvassing (AdCan), a door-to-door data collection in order to update the Master Address File (MAF). The MAF contains important information about all households in the United States. However, the MAF must add and delete addresses every five years based on the habitability of households. Consequently, this process is extremely costly for the Census Bureau. Statistical methodologies are being developed to help predict the changes in habitability using a large number of predictors. This will eliminate the need for the costly AdCan operation. Adragni et al. proposed a methodology called Minimum Average Deviance Estimation or MADE. It is based on the concept of local regression and embeds a sufficient dimension reduction of the predictors. The methodology was developed for response variables from the exponential family distributions and was implemented in R.

The goal of this project is to evaluate the performance of MADE on ultra high dimensional data through simulations. The first step is to parallelize several snippets of the MADE R-script in order to help the code run faster and to analyze the speed-up of these parallelized snippets compared to their serial alternatives. Simulated data with increasing large dimensions will be used to evaluate the runtime under specified hardware setups. In doing this, a limited stress test will be performed to determine how large of a data set UMBC's High-Performance Computer (HPC), maya, can handle. Finally, we will compare two prediction procedures that are devised under MADE. The results of these tests allow evaluating the capabilities of MADE which may help the US Census Bureau to predict the additions and deletions to MAF.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Graduate assistant Elias Al-Najjar was supported during Summer 2015 by UMBC.

#### MORPHOLOGICAL AND BEHAVIORAL EXAMINATION OF OLFACTORY RECOVERY AFTER IRRITANT EXPOSURE IN MICE

<u>Mario Rodriguez</u><sup>2</sup>, Kayla Lemons<sup>1</sup>, Julianna Sun<sup>1</sup>, Chantel Wilson<sup>1</sup>, Ayesha Ibrahim<sup>1</sup>, David Dunston<sup>1</sup>, Wangmei Luo<sup>1</sup>, Tatsuya Ogura<sup>1</sup>, Zi Yang Fu<sup>1</sup>, Weihong Lin<sup>1</sup>
<sup>1</sup>Department of Biology, University of Miami, Coral Gables, Florida 33124
<sup>2</sup>Department of Biological Sciences, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Online access of this abstract is restricted at the request of the Principal Investigator.

This study is supported by NIH/NIDCD DC012831 to Dr. Weihong Lin. Other contributions include the grants given by the Summer Biomedical Training Program (SBTP) via the UMBC College of Natural Mathematics and Science/Graduate School, as well as The Howard Hughes Medical Institute (HHMI) /National Science Foundation (NSF) grants via the University of Miami (UM). I would personally like to express gratitude to mentor Dr. Michael Gaines from the University of Miami and program coordinator Justine Johnson from the SBTP program at UMBC.

### PARALLELIZATION FOR FAST IMAGE RECONSTRUCTION USING THE STOCHASTIC ORIGIN ENSEMBLE METHOD FOR PROTON BEAM THERAPY

REU Site: Interdisciplinary Program in High Performance Computing <u>Fernando Avila-Soto<sup>1</sup>, Alec Beri<sup>2</sup>, Eric Valenzuela<sup>3</sup>, Abenezer Wudenhe<sup>4</sup>,</u> Graduate assistants: Ari Rapkin Blenkhorn<sup>4</sup>, Jonathan S. Graf<sup>5</sup>, Samuel Khuvis<sup>5</sup>, Faculty mentor: Matthias K. Gobbert<sup>5</sup>, Client: Jerimy Polf<sup>6</sup> <sup>1</sup>Department of Computer Science and Mathematics, Muskingum University <sup>2</sup>Department of Computer Science, University of Maryland, College Park <sup>3</sup>Department of Computer Science, California State University, Channel Islands <sup>4</sup>Department of Computer Science and Electrical Engineering, UMBC <sup>5</sup>Department of Mathematics and Statistics, UMBC <sup>6</sup>Department of Radiation Oncology, University of Maryland School of Medicine

Proton beam therapy is becoming increasingly common in the field of cancer treatment because of the advantages over other forms of radiation therapy. This advantage arises from the finite range of the proton beams and the relatively low dosage of radiation upon entering a patient and large spike in dose at the end of the beam range known as the "Bragg peak". By carefully controlling the beam range, the high dose Bragg peak can be used to target tumors while minimizing irradiation of surrounding healthy tissue. Research is currently underway to develop methods to image the proton beam as it passes through the patient as a means of verifying that the Bragg peak is irradiating the tumor as intended. As part of this research, a new computer code has been developed that use the stochastic origin ensemble method to reconstruct an image of the gamma radiation produced by the proton beam. From this image, the behavior of the proton beam in the patient can be studied and verified, i.e., it can be used to predict if the treatment beam is delivering dose correctly at each depth in the patient.

The objective of this research study is to significantly decrease the run time of the given computer code. For the reconstruction algorithm to be useful in medicine, it must be fast and precise, since it is impractical to ask that a patient lie completely still for several minutes. Thus, parallel computing techniques are being applied to the source code for optimizing experimental image reconstruction speed on the UMBC High Performance Computing Facility.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Gabrielle Salib was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Ari Rapkin Blenkhorn, Jonathan Graf, and Samuel Khuvis were supported during Summer 2015 by UMBC.

## Poster Session 1

First Name	Last Name	Program Affiliation	Poster #
Alecia	Achimovich	SBTP Trainee	31*
Trevor	Adriaanse	HPC REU	51*
Tawakalitou	Alabi	SBTP Trainee	57*
Lilian	Anosike	UBM	75*
Alvaro	Arrospide Fletcher	MARC U*STAR Trainee	13
Fernando	Avila-Soto	HPC REU	27*
Tiffany	Bamfo	SBTP Trainee	43*
Courtney	Bass	Independent Research	73
Natithorn	Bhusri	Other	37*
Greg	Brinsley	Independent Research	49
Andrew	Brown	SBTP Trainee	81*
Adam	Byerly	UBM	69*
Grace	Choi	UBM	3*
Binika	Chunara	Other	95
Eric	Cormack	SBTP Trainee	21
Adrian	Davey	HHMI Scholar	5
Erin	DeNardo	HPC REU	15*
Emily	Diaz	Other	65*
Jacob	Dohl	Independent Research	89*
George	Eskandar	HPC REU	79*
Geraldine	Ezeka	Other	61*
Caitlin	Ford	Independent Research	83
Samantha	Furman	MARC U*STAR Trainee	39
Julia	Gao	Independent Research	1
Shyohn	Ghorbanpoor	SBTP Trainee	87
Lindsay	Glang	Independent Research	23
David	Harper	HPC REU	85*
Tessa	Helble	HPC REU	7*
Changling	Huang	HPC REU	47*
Alicia	Khan	MARC U*STAR Trainee	53
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Chloe	Kwon	Independent Research	77
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Melissa	Lucero	MARC U*STAR Trainee	67
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Charlotte	Mann	HPC REU	85*
Monica	Martinez	HPC REU	29
Imani	McLaurin	DREU	91
Briaunna	Minor	SBTP Trainee	101*
Michael	Monaghan	HPC REU	17*
Alexey	Munishkin	HPC REU	17*
Lisa	Nguyen	Independent Research	71
Kamsi	Odinammadu	MARC U*STAR Trainee	9
Colin	O'Hern	Independent Research	55*
DianneMarie	Omire-Mayor	SBTP Trainee	93*
Nicholas	Rojina	HPC REU	15*
Rima	Sakhawala	MARC U*STAR Trainee	19
Carly	Sciandra	Independent Research	97*
Subodh	Selukar	HPC REU	51*
Zoe	Spadaro	SBTP Trainee	57*
Shelbi	Tippett	JCET	33*
Eudorah	Vital	HHMI Scholar	11*
Jessica	Wojtkiewicz	HPC REU	79*
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### SONG PATTERNS IN RESIDENT JAMAICAN YELLOW WARBLERS: A COMPARISON STUDY TO NORTH AMERICAN MIGRATORY YELLOW WARBLERS

Julia Gao<sup>1</sup>, Bernard Lohr<sup>1</sup>, Colin Studds<sup>2</sup> <sup>1</sup>Department of Biological Sciences, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>2</sup>Department of Geography and Environmental Systems, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

I investigated song repertoire and song sharing in a population of resident Yellow Warblers (*Setophaga Petechia*) at Font Hill Nature Preserve, Jamaica in order to compare song patterns of a non-migratory population to previously studied North American migratory populations of this species. Theoretically, as a consequence of year-round residence in an isolated area, and maintaining the same territory for longer periods of time, resident Jamaican yellow warblers should have smaller repertoire sizes but exhibit more song sharing among neighbors. I recorded songs from 3 clusters of 3 neighboring males, for a total of 9 individuals, and analyzed their song patterns using sound spectrograms. I found that resident Jamaican yellow warblers have smaller repertoire sizes with an average of 8.7 song types in comparison to an average of 17 song types in North American migratory populations. Song patterns differed between the two populations of Yellow Warbler. Jamaican birds sang with eventual variety and no differentiation of Type I and Type II singing modes, contrary to patterns in North American populations. Song sharing was also more evident among neighbors than non-neighbors in the Jamaican population.

Thank you to the Smithsonian Institution for funding my trip to Font Hill Nature Preserve in Jamaica, where I conducted my fieldwork, and the Lohr Lab for access to song analysis software.

### GENE EXPRESSION NETWORKS OF HISTONE METHYLTRANSFERASES SET1 AND SET5 IN S. CEREVISIAE

<u>Grace H. Choi</u><sup>1\*</sup>, <u>Rushmie Kulkarni</u><sup>2\*,</sup> DoHwan Park<sup>1</sup>, Erin Green<sup>2</sup> <sup>1</sup>Department of Mathematics & Statistics, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>2</sup>Department of Biological Sciences, UMBC, 1000 Hilltop Circle Baltimore, MD 21250 \* These authors contributed equally to this work

Histone methyltransferases Set1 and Set5 play key roles in the modification of chromatin to regulate gene expression. In 2014, Martin et al. characterized new functional consequences of losing either one or both Set1 and Set5 in budding yeast. This work revealed that both methyltransferases are important for repressing lowly expressed genes near telomeres and retrotransposons. Our study revisits this raw data and performs alternative methods of RNA-seq analysis for gene expression profiling under a Bioconductor/R pipeline and CLC Genomics workbench protocol. After determining significant differentially expressed genes compared to a wild type (WT) strain, we performed hierarchical clustering and correlation analysis between the set 1 $\Delta$ , set 5 $\Delta$ , and set 1 $\Delta$  set 5 $\Delta$  mutants and microarray data of 16 additional strains lacking wellknown chromatin regulators. Clustering based on a Pearson's correlation distance matrix indicates Set5 has an overlapping role with the histone deacetylase Rpd3 and Set1 works in tandem with COMPASS complex components. Preliminary gene ontology (GO) analysis shows significant enrichment for genes involved in sporulation in the set  $1\Delta$  and set  $1\Delta$  set  $5\Delta$  datasets, suggesting an additional function of these histone methyltransferases. Overall, this method of RNA-seq analysis expands our understanding of Set1 and Set5's function and pathway relationships in the regulation of gene expression.

This work was funded, in part, through an Undergraduate Biology Mathematics (UBM) Award from the National Science Foundation under Grant No. DBI 103140, PIs Drs. Leips and Neerchal.

### DEVELOPMENT OF A LOW-COST SENSOR TO DETECT AND QUANTIFY AIRBORNE PM<sub>2.5</sub>

Adrian K. Davey<sup>1,2</sup>, Jared J. Johnson<sup>2</sup>, Jessica Deng<sup>2</sup>, Travis J. McKay<sup>1,2</sup>, Mikhail Y. Kluev<sup>2</sup>, Christopher J. Hennigan<sup>2</sup>

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Fine particulate matter( $PM_{2.5}$ ) imparts detrimental effects on human health; epidemiology studies consistently observe associations between ambient  $PM_{2.5}$  levels and the incidence of premature death. In order to alleviate such health concerns, researchers have implemented and deployed instruments to measure  $PM_{2.5}$  concentrations, increasing coverage in exposed locations. Our lab explores the Sharp Dust Sensor, an extremely low cost (~\$14) aerosol monitor that identifies house dust, cigarette smoke, and other fine particles. This is in contrast to current aerosol instrumentation, which typically costs thousands of dollars (and up).

We utilize Arduino hardware as a microcontroller to operate the Sharp sensor and log its data. We characterized the Sharp sensor in a series of laboratory experiments, including sampling laboratory ambient air, clean air, and rosin smoke. Consistent trends of increased PM<sub>2.5</sub> concentration and voltage were observed with the presence of rosin smoke. We also discerned spikes in voltage similar to those from trials of other researchers investigating the Sharp dust sensor.

The work is ongoing, but future research directions include: (investigation of measures to dampen instrument noise, increase sensitivity, and optimize airflow to the sensor). Ultimately, the sensor will be calibrated using widely accepted (and highly expensive) aerosol sensors, and then deployed for a series of portable characterizations, such as characterizing spatial  $PM_{2.5}$  gradients within the Catonsville area.

This research was supported in part by a grant to UMBC from the Howard Hughes Medical Institute through the Precollege and Undergraduate Science Education Program.

### NUMERICAL EVALUATION OF MINIMUM AVERAGE DEVIANCE ESTIMATION IN ULTRA HIGH DIMENSIONAL POISSON REGRESSION

REU Site: Interdisciplinary Program in High Performance Computing <u>Ely Biggs</u><sup>1</sup>, <u>Tessa Helble</u><sup>2</sup>, <u>George Jeffreys</u><sup>3</sup>, <u>Amit Nayak</u><sup>4</sup>, Graduate assistant: Elias Al-Najjar<sup>2</sup>, Faculty mentor: Kofi P. Adragni<sup>2</sup>, Client: Andrew Raim<sup>5</sup> <sup>1</sup>Department of Applied Mathematics, Wentworth Institute of Technology <sup>2</sup>Department of Mathematics and Statistics, UMBC <sup>3</sup>Department of Mathematics, George Washington University <sup>4</sup>Department of Mathematics, George Washington University <sup>5</sup>US Census Bureau

The second most expensive part of US Census Bureau's decennial census in 2010 was Address Canvassing (AdCan), a door-to-door data collection in order to update the Master Address File (MAF). The MAF contains important information about all households in the United States. However, the MAF must add and delete addresses every five years based on the habitability of households. Consequently, this process is extremely costly for the Census Bureau. Statistical methodologies are being developed to help predict the changes in habitability using a large number of predictors. This will eliminate the need for the costly AdCan operation. Adragni et al. proposed a methodology called Minimum Average Deviance Estimation or MADE. It is based on the concept of local regression and embeds a sufficient dimension reduction of the predictors. The methodology was developed for response variables from the exponential family distributions and was implemented in R.

The goal of this project is to evaluate the performance of MADE on ultra high dimensional data through simulations. The first step is to parallelize several snippets of the MADE R-script in order to help the code run faster and to analyze the speed-up of these parallelized snippets compared to their serial alternatives. Simulated data with increasing large dimensions will be used to evaluate the runtime under specified hardware setups. In doing this, a limited stress test will be performed to determine how large of a data set UMBC's High-Performance Computer (HPC), maya, can handle. Finally, we will compare two prediction procedures that are devised under MADE. The results of these tests allow evaluating the capabilities of MADE which may help the US Census Bureau to predict the additions and deletions to MAF.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Graduate assistant Elias Al-Najjar was supported during Summer 2015 by UMBC.

### ROLE OF ECDYSONE IN THE MIGRATION OF BORDER CELLS IN *DROSOPHILA MELANOGASTER* EGG CHAMBERS

### Kamsi Odinammadu, Neus Sanchez Alberola, Jinal Sheth, Michelle Starz-Gaiano Department of Biological Sciences, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Cell migration is an essential mechanism during animal development. Understanding how cells migrate can help build information that future generations can use in the fight against birth defects and diseases like cancer. As in humans, steroid hormones in Drosophila melanogaster (fruit flies) control the timing of key developmental events, including cell movements, so it is important to investigate how these hormones signal. The goal of this project is to study the role of the steroid hormone Ecdysone in the border cells of fruit fly egg chambers. Border cells are a cluster of motile cells that must migrate during egg development to fulfill their functions. Steroid hormone signaling controls the timing of when border cells exit from the epithelium at the anterior end of the egg chamber and move to the oocyte. Work from multiple labs has identified several factors that are regulated by steroid hormone signaling, such as the role of the protein Abrupt in signaling, and cell adhesion regulators. We have identified many other potential downstream targets of ecdysone signaling through expression analysis. Through genetic experiments, we are determining which of these targets most significantly contribute to cell migration. Prior work has suggested that one of the potential target genes found,  $PH4\alpha EFB$ (Prolyl-4-Hydroxlase alpha, Embryonic Fat Body) may play a role in border cell migration. Mutations that cause an abnormal phenotype are being further characterized. These results will inform us about the important signaling effectors downstream of ecdysone steroid hormone in cell migration. Gaining knowledge about these effectors will help with understanding how similar pathways function.

This investigation was supported in part by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences.

#### MAP1B IMPACTS ON NEURULATION AND MICROTUBULE STABILITY

Eudorah Vital, Jonathan Werner, Pradeepa Jayachandran<sup>\*</sup>, Valerie Olmo<sup>\*</sup>, Stephanie Sanchez<sup>\*</sup>, Elim Hong, Rebecca McFarland, Neus Sanchez- Alberola, Rachel Brewster Department of Biological Sciences, UMBC, 1000 Hilltop Circle, Baltimore, MD 212150

Brain development is a stepwise process that begins with neurulation. It is the process by which the neural tube develops, the precursor to the brain and spinal cord. Disrupting the intricate process of neurulation can result in mild to severe neural birth defects. An important and conserved event in neurulation is neural convergence extension (NCE) of the neural ectoderm. During NCE, neuroepithelial cells elongate mediolaterally and migrate towards the midline, thus narrowing and lengthening the neural plate. An important cellular component that drives NCE are microtubules (MTs). MTs are dynamic cytoskeletal tracts that drive tissue morphogenesis. Insufficient regulation of microtubule dynamics during neurulation is associated with neural tube defects in model organisms. MTs shorten, lengthen, and stabilize at the instruction of intrinsic and extrinsic factors to shape the tissues using cellular processes that are poorly understood. One such process is regulation by Microtubule Associated Proteins (MAPs), which bind directly to microtubules. Most MAPs control dynamics and stability. Specifically, Map1b temporally modulates MT polymerization and axon elongation, crucial aspects of early nervous system development.

In the direction of better understanding Map1b and its impacts, MO and Dominant Negative (DN) constructs were used to generate Map1b loss of function (LOF) phenotypes in zebrafish embryos. We found that depleting Map1b with MOs delayed NCE. Histological examination of the MO experiments showed that Map1b depletion caused destabilization in microtubule lattices and altered cell morphology during NCE. Our results are congruent with others that markedly implicate Map1b as a key microtubule regulator during neural tube morphogenesis.

After the alleged invalidation of MOs in recently published paper, we began using RNA Dominant Negatives (DN) to knock-out Map1b. Preliminary results from our dominant negative study are forthcoming, however, we anticipate agreement with the MO study.

Thank you to Dr. Rachel Brewster, our mentor Stephanie Sanchez, and our lab members for their guidance and contributions. Also, thank you to the Meyerhoff scholars program, and the Howard Hughes Undergraduate Scholars Program.

Notes:

\*These authors contributed equally to this work

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#### CLUSTERING TEXT DATA WITH A TANDEM OF BIRCH AND K-MEANS

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The process of data clustering consists of grouping data such that elements in each group are more similar to each other than to those in other groups. Data clustering is used in a broad range of areas such as information retrieval, bioinformatics, very-large-scale integration, data mining, text mining and image analysis to name just a few. Text data is usually transformed in high dimensional and sparse vectors. High dimensional data clustering is a useful and practical approach for exploratory data mining. A possible approach to clustering high dimensional data is the k-means algorithm. However, k-means requires that an initial partition is supplied. The clustering scheme Balanced Iterative Reducing and Clustering using Hierarchies (BIRCH) requires a single scan of the data set in order to provide such partition. We sought to determine the results of applying a tandem of BIRCH followed by k-means to the well-known and publicly available Classic3 data set. This dataset consists of 3 different document collections: CISI (1460 information science abstracts), CRAN (1398 aerodynamics abstracts), and MED (1033 medical abstracts). We implemented BIRCH and k-means in Java and analyzed the quality of the partitioned dataset at each step. Different orderings of the data set were partitioned so as to determine the stability of this clustering scheme. We also constructed confusion matrices to visualize the partitions generated by BIRCH and k-means. Our results suggest that this scheme is stable and effective at clustering high-dimensional and sparse text data. Further research will be done on clustering actual data sets originating from additional text collections.

This investigation was supported by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences.

#### IMPACT OF CALCIUM STORE OVERLOAD ON ELECTRICAL DYNAMICS OF CARDIAC MYOCYTES

REU Site: Interdisciplinary Program in High Performance Computing <u>Amanda M. Alexander<sup>1</sup>, Erin K. DeNardo<sup>2</sup>, Eric Frazier III<sup>3</sup>,</u> <u>Michael McCauley<sup>4</sup>, Nicholas Rojina<sup>5</sup></u> Graduate assistant: Zana Coulibaly<sup>4</sup> Faculty mentor: Bradford E. Peercy<sup>4</sup>, Client: Leighton T. Izu<sup>6</sup>

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Heart disease is the leading causes of mortality in the United States. One cause of heart arrhythmia is calcium mishandling in cardiac muscle cells. We are presenting a mathematical model of the mechanism by which calcium waves propagate through cardiac muscle, or cardiomyocytes. This mechanism involves calcium being released from the sarcoplasmic reticulum (SR) through calcium release units (CRUs) in sparks. These sparks can cause other CRUs to release calcium, producing waves of calcium throughout the cell. The mathematical model is coded in C and run using parallel computing to efficiently generate simulations of the model; Matlab is utilized to create images indicating the calcium concentration throughout a cardiac cell with respect to time. Our model accounts for changes in the calcium concentration of the SR, the effects of buffers in the SR, particularly calsequestrin and other SR buffers, and the effects of voltage across the cell membrane. We have found that incorporating a dynamic SR calcium concentration causes the flux of calcium through open CRUs to taper off over the duration of the CRU firing, ultimately lowering the likelihood of waves to propagate. Likewise, including the effects of calcium buffers in the SR decreases the free calcium concentration, again affecting the likelihood of waves to propagate. Additionally, voltage-gated channels are utilized to examine the impact of calcium dynamics on voltage across the membrane.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing hpcreu.umbc.edu in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos.~CNS--0821258 and CNS--1228778) and the SCREMS program (grant no.~DMS--0821311), with additional substantial support from UMBC. Co-author Michael McCauley was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Zana Coulibaly was supported during Summer 2015 by UMBC.

#### COMPARISON OF PERFORMANCE ANALYSIS TOOLS FOR PARALLEL PROGRAMS APPLIED TO CombBLAS

REU Site: Interdisciplinary Program in High Performance Computing <u>Wesley Collins<sup>1</sup></u>, <u>Daniel T. Martinez<sup>1</sup></u>, <u>Michael Monaghan<sup>2</sup></u>, <u>Alexey A. Munishkin<sup>3</sup></u>, Graduate assistants: Ari Rapkin Blenkhorn<sup>1</sup>, Jonathan S. Graf<sup>4</sup>, Samuel Khuvis<sup>4</sup>, Faculty mentor: Matthias K. Gobbert<sup>4</sup>, Client: John C. Linford<sup>5</sup> <sup>1</sup>Department of Computer Science and Electrical Engineering, UMBC, <sup>2</sup>College of Earth and Mineral Sciences, The Pennsylvania State University, <sup>3</sup>Jack Baskin School of Engineering, Department of Computer Engineering, UCSC, <sup>4</sup>Department of Mathematics and Statistics, UMBC, <sup>5</sup>ParaTools, Inc.

Performance analysis tools, or profilers for short, can be powerful tools for high performance computing. When a computer program is running slowly, it may be difficult to tell, where the bottleneck is located in the code, in particular if the code is a parallel program. By breaking it down to how long the CPUs are taking on each process (profiling) or showing when events take place on a timeline over the course of running a program, a performance analysis tool can tell the programmer exactly, where the computer is running slowly. With this information, the programmer can focus on these performance "hotspots," and the code can be optimized to run faster.

We compare the performance analysis tools TAU, ParaTools Threadspotter, Intel VTune, Scalasca, HPCToolkit, Score-P, when applied to the example of CombBLAS (combinatorial BLAS), a C++ algorithm in the GraphBLAS set of graph algorithms using BLAS (Basic Linear Algebra Subroutines). Using these results, we improve the implementation of CombBLAS and show performance data obtained on the distributed-memory cluster maya in the UMBC High Performance Computing Facility.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-authors Wesley Collins and Daniel Martinez were supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Ari Rapkin Blenkhorn, Jonathan Graf, and Samuel Khuvis were supported during Summer 2015 by UMBC.

### INVESTIGATING RLS1 LOCALIZATION AND THE EVOLUTIONARY ORIGINS OF CELLULAR DIFFERENTIATION

#### <u>Rima Sakhawala</u>, Jose Ortega, Stephen Miller Department of Biology, UMBC, 1000 Hilltop Circle, Baltimore, Maryland 21250

The evolution of cellular differentiation was a key step in the origin of complex life, but little is known about the molecular mechanisms that made this developmental innovation possible. Volvocine green algae are good model organisms to study this question because they are closely related yet have very different developmental programs. In particular, Chlamydomonas reinhardtii is unicellular, and Volvox carteri is multicellular with two different cell types: reproductive gonidia and motile somatic cells. In V. carteri, RegA is responsible for repressing growth and reproduction in its somatic cells, keeping them terminally differentiated. RegA contains a conserved region, the VARL (Volvocine Algae RegA Like) domain that is found in several homologs in both V. carteri and C. reinhardtii. RLS1 is the closest C. reinhardtii homolog of RegA. RLS1 mRNA is more abundant when cells are stressed by nutrient or light deprivation, but little is known about this gene or the protein it encodes. Learning more about RLS1 function may provide important insights into the origins of RegA and how it represses reproduction. To this end, our immediate goal is to learn more about the accumulation and localization of the RLS1 protein. In order to study protein accumulation and localization during the C. reinhardtii life cycle, we are making a construct that expresses mCherry-tagged RLS1 protein, so that we can determine accumulation in vivo by fluorescence. The mCherry fragment was generated by PCR and will be ligated using a unique restriction site into a plasmid containing the RLS1 gene. The completed construct will be transformed into C. reinhardtii for fluorescence analysis. Follow up studies will involve other constructs that overexpress RLS1 or that eliminate its function, and together our work should help us better understand RLS1 and ultimately, the evolutionary origins of RegA.

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#### GEL ANALYSIS OF THE HIV-1 5' UTR AT NMR CONCENTRATIONS

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HIV-AIDS has long been and remains one of the most devastating diseases on earth. Fundamentally, the disease is incurable, and treatment can at best force the virus into dormancy within T-cells. Modern treatments use a cocktail of drugs to inhibit the virus in many parts of the viral life cycle. If future treatments could eliminate the need for a cocktail, there would be fewer adverse side affects, lower cost, and more effective treatment.

Our research focuses on the structural components of the HIV-1 RNA genome. Specifically, we hope to solve the structure of the 5'-untranslated region (5' UTR) of the genome. This region of the genome is highly conserved, meaning that mutations in this region are not sustainable for the virus, and prevent a continuation of that virus' life. Thus, targeting this region for treatment would inhibit many essential elements of viral reproduction, and could eliminate the need for a cocktail of drugs. Within the cytosol, the genomic RNA exists as an equilibrium between its monomer and dimer conformations. While the dimer is essential for packaging, the monomer is translated into the viral proteins. This dimerization occurs at the 5' UTR. We hope to use nuclear magnetic resonance (NMR) techniques to elucidate the monomer conformation. To shift the monomer-dimer equilibrium, we have executed a number of truncations at different sites on the 5' UTR. These truncated constructs are run on gels to test the rate and equilibrium constants of dimerization. In particular, NMR requires highly concentrated, very pure samples of construct. As such, our gels have been testing the monomer-dimer equilibration rate and equilibrium constants at very high concentrations of construct. We are in the midst of creating and testing a number of these constructs.

This research was funded by NIH/NIGMS grant *1P50GM103297*, Summer Biomedical Training Program (*SBTP*), and was conducted at the Howard Hughes Medical Institute at UMBC with support in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. We would also like to thank our research team Seungho Choi, Hannah Carter, Aishwarya Iyer, and Shyohyn Ghorbanpoor for their assistance.

#### DETERMINATION OF THE HIV-1 REV RESPONSE ELEMENT STRUCTURE BY NUCLEAR MAGNETIC RESONANCE

Lindsay Glang<sup>1</sup>, Andrew Brown<sup>2</sup>, Katherine Grace Canham<sup>3</sup>, Roald Teuben<sup>1</sup>, Geraldine Ezeka<sup>1</sup>, Jan Marchant<sup>1</sup>, and Michael F. Summers<sup>1</sup> <sup>1</sup>Howard Hughes Medical Institute, Department of Chemistry and Biochemistry, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>2</sup>Department of Chemistry and Biochemistry, University of Maryland College Park, MD, 20743 <sup>3</sup>Department of Biological Sciences, Towson University, 8000 York Road, Towson, MD 21252

The Rev response element (RRE) is a noncoding region of the HIV-1 genome associated with nuclear export of complete, unspliced viral RNA. It acts as a scaffold for the accessory protein Rev, forming a complex that is recognized by host nuclear export machinery. We are working to characterize the three-dimensional structure of the RRE because it will offer unique insights and a better understanding of the mechanisms by which it operates.

Nuclear Magnetic Resonance (NMR) spectroscopy has been utilized for the determination of RNA structures in physiologically relevant solution conditions. However, it is generally applied to small structures below forty nucleotides in length. NMR spectra of large RNAs, such as the 233 nucleotide RRE, are extremely difficult to analyze due to broad signals and severe chemical shift overlap. We are utilizing a number of strategies to combat these difficulties. Based on computational predictions, we initially created an array of small RRE fragments, which were compared to the full-length spectra. Using this data, we were able to identify specific elements that allow us to segment the RNA. The segments are then annealed back together, and can be used in conjunction with different deuterium-labeled nucleotide schemes. Deuterium-labeled nucleotides do not show peaks in the NMR spectra, therefore giving a simplified spectra and providing a full-length structure that allows access to sections of the RRE that are typically more difficult to distinguish.

The use of these techniques will contribute to the determination of the secondary structure of the RRE, and ultimately provide the three-dimensional structure.

I would like to acknowledge the NIH/NIGMS # P50GM103297, and the Howard Hughes Medical Institute.

### INTIMATE PARTNER VIOLENCE: THE EFFECTS OF PERPETRATOR CHARACTERISTICS ON TREATMENT ENGAGEMENT AND OUTCOME

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Perpetrators of intimate partner violence tend to blame others for their problems. These attitudes can be very problematic as they can be associated with less motivation to change and non-compliance with treatment, both of which can be exacerbated by being court-mandated to treatment, which the majority are. For these reasons, non-compliance is one of the biggest challenges for treatment programs. In an effort to increase compliance, researchers have turned to readiness to change. Readiness to change is a composite score obtained from the Transtheoretical Model of Behavior Change that determines the extent to which one is ready to change their problematic behavior. If we can better understand and measure readiness to change, we can predict treatment engagement as well as treatment outcome.

The current study investigates readiness to change as a predictor of treatment engagement and outcome in using archival data from a community-based counseling program for male perpetrators of intimate partner abuse. It is predicted that readiness to change will be positively related to treatment engagement and negatively related to criminal recidivism. Additionally, referral status, antisocial and borderline personality characteristics will moderate these relationships. At program intake, readiness to change, demographics, referral source, and borderline and antisocial personality traits were assessed. During treatment, clients (N = 197) completed measures of working alliance and group cohesion, and their therapists completed ratings of homework compliance and working alliance. Criminal recidivism data was gathered from public criminal records for the two years after scheduled completion of treatment.

Results suggest that having a higher readiness to change is beneficial for court-ordered individuals and individuals with high borderline and antisocial characteristics because it helps them have better treatment engagement and lower recidivism. Given these findings, supplementary treatment, such as motivational interviewing, should be provided for individuals who have high borderline and antisocial characteristics.

These results were obtained as part of the Summer Biomedical Training Program in the Department of Psychology at the University of Maryland, Baltimore County. This research is funded by Princeton University, with additional support from University of Maryland Baltimore County and Christopher Murphy.

### PARALLELIZATION FOR FAST IMAGE RECONSTRUCTION USING THE STOCHASTIC ORIGIN ENSEMBLE METHOD FOR PROTON BEAM THERAPY

REU Site: Interdisciplinary Program in High Performance Computing <u>Fernando Avila-Soto<sup>1</sup>, Alec Beri<sup>2</sup>, Eric Valenzuela<sup>3</sup>, Abenezer Wudenhe<sup>4</sup>,</u> Graduate assistants: Ari Rapkin Blenkhorn<sup>4</sup>, Jonathan S. Graf<sup>5</sup>, Samuel Khuvis<sup>5</sup>, Faculty mentor: Matthias K. Gobbert<sup>5</sup>, Client: Jerimy Polf<sup>6</sup> <sup>1</sup>Department of Computer Science and Mathematics, Muskingum University <sup>2</sup>Department of Computer Science, University of Maryland, College Park <sup>3</sup>Department of Computer Science, California State University, Channel Islands <sup>4</sup>Department of Computer Science and Electrical Engineering, UMBC <sup>5</sup>Department of Mathematics and Statistics, UMBC <sup>6</sup>Department of Radiation Oncology, University of Maryland School of Medicine

Proton beam therapy is becoming increasingly common in the field of cancer treatment because of the advantages over other forms of radiation therapy. This advantage arises from the finite range of the proton beams and the relatively low dosage of radiation upon entering a patient and large spike in dose at the end of the beam range known as the "Bragg peak". By carefully controlling the beam range, the high dose Bragg peak can be used to target tumors while minimizing irradiation of surrounding healthy tissue. Research is currently underway to develop methods to image the proton beam as it passes through the patient as a means of verifying that the Bragg peak is irradiating the tumor as intended. As part of this research, a new computer code has been developed that use the stochastic origin ensemble method to reconstruct an image of the gamma radiation produced by the proton beam. From this image, the behavior of the proton beam in the patient can be studied and verified, i.e., it can be used to predict if the treatment beam is delivering dose correctly at each depth in the patient.

The objective of this research study is to significantly decrease the run time of the given computer code. For the reconstruction algorithm to be useful in medicine, it must be fast and precise, since it is impractical to ask that a patient lie completely still for several minutes. Thus, parallel computing techniques are being applied to the source code for optimizing experimental image reconstruction speed on the UMBC High Performance Computing Facility.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Gabrielle Salib was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Ari Rapkin Blenkhorn, Jonathan Graf, and Samuel Khuvis were supported during Summer 2015 by UMBC.

#### RELIABILITY OF ACCELEROMETER-BASED GAIT ANALYSIS: PROVIDING A BASIS FOR COMPARISON

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Just as wearable technology is becoming prevalent in society, the possibility for its applications within the realm of healthcare has also experienced significant growth. One such application example is accelerometer-based gait analysis testing. Gait analysis testing is the technique used to both assess the severity of diseases that greatly impact gross motor skills, such Alzheimer's and Parkinson's Disease, and provide treatment options for traumas such as stroke. And yet, this method of gait testing has been underutilized due to a costly, time-consuming process that more often than not yields unclear and unreliable data. However, recent modern wearable fitness devices have achieved a degree of accuracy and reliability which may make them ideal for conducting at-home gait analysis testing as both a low cost and time-saving alternative for patients and clinicians. For our study we will compare data obtained from clinical devices used for gait analysis with non-clinical devices, such as mobile phones and wearable technology, in order to attest to the efficacy of at-home accelerometer-based gait analysis. Our method involves obtaining step counts from five different devices (APDM, Axivity, Actigraph, AndroSensor, and Fitbit) attached at the waist of participants as they walk on a treadmill for four minute intervals at speeds resembling those of patients with impaired gross motor skills (1.3, 1.1, and 0.9ms). Our research aim is to identify the reliability of each device, their limitations and or advantages, and to provide baseline data for accelerometer-based gait analysis testing.

The work of Monica Martinez is supported in part by the Distributed Research Experiences for Undergraduates (DREU) program, a joint project of the CRA Committee on the Status of Women in Computing Research (CRA-W) and the Coalition to Diversify Computing (CDC), which is funded in part by the NSF Broadening Participation in Computing program (NSF CNS-0540631).

### CHARACTERIZING MATRIX'S ROLE IN PACKAGING tRNA<sup>Lys3</sup> IN HIV-1 VIRIONS THROUGH SITE-DIRECTED MUTAGENESIS OF BASIC PATCH RESIDUES

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Upon infection of a CD-4 cell, the RNA genome of HIV is reverse transcribed into DNA. The initiation of this process requires a host cell tRNA<sup>Lys3</sup> to act as a primer and bind to the primer binding site of the genomic RNA, allowing for elongation of the complementary strand. After non-specific integration and subsequent transcription of the intermediate, the unspliced variant of the resultant RNA can be translated into gag and gag-pol proteins. The N-terminal of this polyprotein is functionally characterized as the matrix domain which is quintessential for plasma membrane targeting and binding as well as the assembly and budding of immature virion. Further, past studies have shown that the matrix domain binds to RNAs, the majority of which are tRNAs, via the same highly basic region. The previously mentioned tRNA<sup>Lys3</sup>, though found at a relatively low concentration in the cell, binds with a high frequency. This suggests that matrix may play an integral role in packaging tRNA for further use during reverse transcription.

Based on these previous reports, our goal is to structurally characterize matrix and tRNA interactions through the use of Electrophoretic Mobility Shift Assays (EMSA). Specific tRNA-matrix binding has been further supported by EMSA. In order to determine which residues are important for binding, we have constructed mutants of the matrix protein at residues which have been previously reported to be integral for specific non-promiscuous binding to PI(4,5)P<sub>2</sub> containing membranes. The mutant construct K29A did not show a significant decrease in tRNA binding while the K29, 31A construct needs to be studied further. Direct structural implications of the binding will be studied via HSQC in the future.

This research was funded by both the Howard Hughes Medical Institute (HHMI), HHMI's Exceptional Research Opportunities (EXROP) fellowship and, in part, by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences. Further, we would like to thank Dr. Michael Summers, Christy Gaines, Justine Johnson and the Summer Biomedical Training Program (SBTP) for their unwavering support.

### REMOTE SENSING MONITORING OF CANADIAN WILDFIRE SMOKE AND ITS IMPACT ON BALTIMORE AIR QUALITY

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High spatial and temporal resolution Elastic *light detection and ranging* (lidar) measurements allows to monitor long-range transport of particulates, such as dust and smoke, that impact local and regional air quality. These lidar measurements enhance current knowledge and understanding on how vertical layering and long range transport of natural and anthropogenic particle pollution may alter the relationship between column aerosol optical depth and surface particle pollution concentrations. The impact of a strong haze event in June 9-11, 2015 is examined. Particle pollution associated to this event yielded a 245% increase in aerosol optical depth values compared to the average mean June values for the last decade. We present how air mass back trajectory analysis, aerosol intensive and extensive parameters from lidar, sun-photometer and satellite observations revealed the presence of Canadian wildfire smoke impacting the Baltimore air quality.

The research is supported by NOAA-CREST/CCNY Foundation CREST Grant-NA11SEC481004.3 and the Joint Center for Earth Systems Technology.
#### GROUNDING COST IN LAPAROSCOPIC SURGERY

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Attending surgeons often physically and verbally instruct residents on how to understand the laparoscopic video throughout a laparoscopic surgery. Our purpose is to identify the phases of surgery where residents require more explicit instructions to make progress in a surgery in order to discuss ways to technologically support laparoscopic surgery and OR-based training. We divided one particular procedure, a laparoscopic cholecystectomy, into four phases: preparation, gallbladder isolation, gallbladder removal, and cleanup. We identified the number of utterances and length of operative time for every phase. A non-parametric Friedman test of differences among repeated measures was conducted to compare the number of utterances across the four phases. Overall, there were significant differences among the frequencies of utterances across the phases of surgery (chi-square = 19.08, p < 0.001). The post-hoc comparisons showed that the frequency of utterances was significantly higher in Phase 2 and 3 at a confidence level of 95%. However, there was no significant difference between Phase 2 and 3. We further conducted an ANOVA with repeated measures with a Greenhouse-Geisser correction to compare the length of operative time over the phases. The test results show that the mean operative times for phases were statistically significantly different (F (2.117, 19.055) = 6.348, p = 0.007). The post-hoc tests with Bonferroni correction show that Phase 1 is significantly shorter than Phase 2 and 3. Our results indicate that Phase 2 and 3 requires more effort and time for surgeons to develop and update common ground in order to proceed in the surgery. Our study highlights the needs for interactive instructional systems in Phase 2 and 3 in order to minimize the collaborative efforts. The design can focus on transforming contextualized guidance into visual cues on the videos to increase the efficient understanding of utterances.

This work was sponsored by NSF Grant IIS – 1422671.

#### COPPER BIOREMEDIATION USING GENETICALLY ENGINEERED ESCHERICHIA COLI

<u>Alex Kuznetsov<sup>1</sup></u>, <u>Natithorn Bhusri<sup>1</sup></u>, UMBC iGEM team<sup>2</sup>, Cynthia Wagner<sup>3</sup>, Stephen Freeland<sup>4</sup> <sup>1</sup>Department of Chemistry and Biochemistry, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>3</sup>Department of Biology, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>4</sup>Department of Interdisciplinary Studies, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

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Copper is a major pollutant in a variety of freshwater ecosystems. When copper is oxidized from  $Cu^+$  to  $Cu^{2+}$ , it often produces a free radical known as a reactive oxygen species (ROS), which is capable of severely damaging biological molecules. *E. coli* have the ability to uptake copper, but after a certain threshold, the copper becomes toxic to the cell. Due to the toxicity of copper, *E. coli* quickly saturate and are unable to uptake more than a small amount of copper.

Our goal is to increase the efficiency of copper uptake in *E. coli* for the purpose of bioremediation in freshwater ecosystems. We engineered *E. coli* to express the yeast CUP1 gene in an attempt to increase copper tolerance. CUP1 encodes a metallothionein protein that binds 11 copper atoms, thereby preventing formation of the ROS. In addition, metallothionein detoxifies hydroxyl radicals with its cysteine groups.

Through the use of growth curves and an assay to measure copper uptake, we will present our preliminary data on *E.coli* transformed with the CUP1 gene as our initial attempt to create a bacterial strain that has a higher resistance to copper toxicity.

The UMBC iGEM Team would like to acknowledge the UMBC Student Government Association, the UMBC College of Natural and Mathematical Sciences, UMBC Biology Department and UMBC Chemistry and Biochemistry Department for their financial support without which our project would not be feasible. We would also like to acknowledge Dr. Stephen Mang for his support with copper measurement.

# SKELETAL MUSCLE ATROPHY MODEL: INTEGRATING INSULIN INTO THE FOXO-1 MODEL

#### Samantha Furman, Dr. Bradford E. Peercy

Department of Mathematics and Statistics, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Skeletal muscle atrophy is the degradation of muscle cells due to either aging, or as a result of a medical ailment such as cancer, diabetes or heart disease. The class of transcription factors, Foxo-1, are important in atrophy because the nuclear concentration of Foxo-1 controls muscle degrading proteins and determines the rate of muscle atrophy or decay. Previous research has given parameters for the rates of (de)phosphorylation with a steady insulin value. I modeled the effects of external stimuli, such as insulin like growth factor (IGF-1) on the phosphorylation of Foxo-1 and it's effects on the movement of dephosphorylated Foxo-1 inside and phosphorylated Foxo-1 outside of the nucleus. I was able to link a previous model of insulin/IGF-1 activation of the phosphorylation enzyme Akt with our model of Akt phosphorylation of Foxo-1 to quantify the insulin/IGF-1 impact on the Foxo-1 nuclear cytoplasmic ratio. I conducted this research using differential equations, non-dimensional analysis, parameter optimization and simulation using dynamical systems software, primarily Matlab. This system is a prototype of other transcription factor nuclear translocation systems that will benefit from our mathematical analysis.

This investigation was supported in part by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences. Also, thank you to my mentor, Dr. Bradford E. Peercy, and our collaborators, Dr. Martin Schneider and Sarah Greene.

#### INVESTIGATING DIMERIZATION MECHANISMS IN THE 5'-UNTRANSLATED REGION IN HUMAN IMMUNODEFICIENCY VIRUS

#### <u>Ae Lim(Ally) Yang</u>, Jessica Zaki, Michelle Seu, Thao Tran, Michael F. Summers Department of Chemistry and Biochemistry, Howard Hughes Medical Institute at UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

There are two types of Human Immunodeficiency Virus (HIV), HIV-1 and HIV-2, and both viruses cause Acquired Immunodeficiency Syndrome (AIDS), which has taken millions of lives. A recent proposed model of HIV-1 5' leader (5'-L) dimerization shows the dimerization initiation site (DIS) stem-loop within the intact leader is necessary in retroviral replication cycle. In contrast to HIV-1 model, HIV-2 studies suggest that the DIS is dispensable for HIV-2 leader dimerization. According to phylogenetic and structural biology studies, both HIV-1 and HIV-2 leaders contain DIS stem-loops with similar palindromic sequences. To our surprise, other studies of HIV-2 suggest that the DIS is dispensable for HIV-2 leader dimerization. Hence, we probed for the role of the DIS in the HIV-2 leader dimerization mechanism by conducting time-dependent and pH-dependent dimerization assays.

We introduced different mutations at the DIS of HIV-2 leaders and probed for the dimerization behavior of these mutants using native gel electrophoresis. We have found that the mutant containing an impaired DIS palindrome (5'-LCCA) and the mutant containing stem loop that has been replaced with the DIS of HIV-1 (5'-LHIV-1 loop) both show more dimer as the incubation time increases. Interestingly, the 5'-LCCA mutant induces more dimer as pH in the incubation buffer increases, whereas the 5'-LHIV-1 loop shows the opposite trend. Our increased understanding of the structural science of HIV-2 genome will allow for greater possibilities to aid in the anti-retroviral drug development.

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#### THE BINDING OF FIV MA TO MIMETIC MEMBRANES

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The feline immunodeficiency virus (FIV) is a lentivirus that weakens the immune system of the infected cat, similar to the effects of the human immunodeficiency virus in humans. The assembly process is vital to the retroviral replication cycle because the Gag polyprotein (Gag) is targeted to the plasma membrane of the host cell during this stage. The component of Gag that mediates its transportation and interaction with the plasma membrane is the matrix domain (MA). The proposed extended lipid binding model demonstrates how HIV-1 MA binds to the plasma membrane. The limitations in this proposed model are the purpose behind our studies: truncated lipids were used in this study, but we strive to use the native lipid to better characterize binding. This work investigates how FIV MA operates in targeting and binding to the lipid phosphatidylinositol-(4,5)-bisphosphate [PI(4,5)P<sub>2</sub>] with the use of liposomes as mimetic membranes. Our reasoning behind studying the virus in cats is that, like HIV Gag, FIV Gag binds to PI(4,5)P<sub>2</sub>, many cats are already infected with the virus so the risk of unnecessary harm for research purposes is reduced, and unlike simians, it is inexpensive to house and maintain cats during study. Nuclear magnetic resonance spectroscopy (NMR) is used to qualitatively analyze the binding interaction between FIV MA and PI(4,5)P<sub>2</sub>. Comparison of membrane targeting in FIV MA and HIV-1 MA may support application of household cats as animal models for the treatment of HIV. In addition to studying the assembly process, great focus is placed on efficiently preparing protein for NMR studies by developing a new concentrating protocol.

This study was supported in part by NIH/NIAID 5R37AI030917, HHMI, and the Summer Biomedical Training Program.

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#### PERFORMANCE STUDIES OF THE BLOSSOM V ALGORITHM

REU Site: Interdisciplinary Program in High Performance Computing <u>Changling Huang</u><sup>1</sup>, <u>Christopher C. Lowman</u><sup>2</sup>, <u>Brandon E. Osborne</u><sup>3</sup>, <u>Gabrielle M. Salib</u><sup>4</sup>, Graduate assistants: Ari Rapkin Blenkhorn<sup>4</sup>, Jonathan S. Graf<sup>5</sup>, Samuel Khuvis<sup>5</sup>, Faculty mentor: Matthias K. Gobbert<sup>5</sup>, Clients: Tyler Simon<sup>6</sup> and David Mountain<sup>6</sup> <sup>1</sup>Department of Mathematics and Department of Computer Science, Rutgers University <sup>2</sup>Department of Mathematics, University of Maryland, College Park <sup>3</sup>Department of Physics and Astronomy, Austin Peay State University <sup>4</sup>Department of Computer Science and Electrical Engineering, UMBC <sup>5</sup>Department of Mathematics and Statistics, UMBC <sup>6</sup>Laboratory for Physical Sciences

The Blossom V algorithm is an important algorithm used in graph theory to compute a perfect matching of minimum cost of a graph. Graph theory allows for effective modeling of real-world scenarios. With growing amounts of data, the fast speed of algorithms becomes imperative to their efficiency. Performance studies were run on the maya cluster in the UMBC High Performance Computing Facility to investigate the performance of the algorithm on graphs of various sizes and orders. Various time measurements and total memory usage were recorded for the different graphs. Several memory profilers, such as Valgrind, were used to determine memory usage. Systematic studies for a variety of sizes and orders are used to analyze the total execution time and memory usage of the algorithm. The execution time increases steadily with the size and order of the graphs, and we can pinpoint the location of major portions of execution time. Also memory usage increases steadily with the size and order of the graphs, as memory usage is largely attributed to the size of the structures used to store the vertices and edges of the graph. The results of the performance studies indicate areas of the algorithm that will benefit from potential parallelization. Future research may include development of a parallel implementation of the Blossom V algorithm in order to improve execution time. Furthermore, potential techniques to reduce memory consumption should be explored.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Gabrielle Salib was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Ari Rapkin Blenkhorn, Jonathan Graf, and Samuel Khuvis were supported during Summer 2015 by UMBC.

#### MICROWAVE LYSING AND FRAGMENTATION OF NEISSERIA GONORRHOEAE

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Common techniques for bacterial DNA isolation and fragmentation are often costly and time-consuming. The cost associated with DNA isolation is associated with the number of reagents necessary for DNA purification. By using standard microwaves along with equilateral gold triangles deposited on microscope slides, this process becomes expedited and reagent-less. The equilateral triangles help to focus the microwaves directly onto the sample, thus allowing for localization of energy and an increase in the rate of cell lysis and DNA fragmentation. The overarching goal of this project is to use Microwave-Accelerated Metal-Enhanced Fluorescence (MAMEF)-based assay for detection of *Neisseria Gonorrhoeae* as well as other pathogenic organisms. MAMEF is a quick and inexpensive detection method compared to other common methods such as polymerase chain reaction (PCR). The current project aim is to develop a rapid, microwave-based method to isolate and fragment DNA from organisms with similar and different cell wall architecture. The development of a rapid DNA isolation and fragmentation method coupled with MAMEF provides a novel, rapid and sensitive platform towards the detection of microbial pathogens.

# STATISTICAL ANALYSIS OF A CASE-CONTROL ALZHEIMER'S DISEASE: A RETROPECTIVE APPROACH WITH SUFFICIENT DIMENSION REDUCTION

REU Site: Interdisciplinary Program in High Performance Computing <u>Trevor V. Adriaanse<sup>1</sup></u>, <u>Meshach Hopkins<sup>2</sup></u>, <u>Rebecca Rachan<sup>3</sup></u>, <u>Subodh R. Selukar<sup>4</sup></u>, Graduate Assistant: Elias Al-Najjar<sup>2</sup> Faculty Mentor: Kofi P. Adragni<sup>5</sup>, Client: Nusrat Jahan<sup>6</sup>

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Alzheimer's Disease is a neurological disorder chiefly present in the elderly that affects functions of the brain such as memory and logic, eventually resulting in death. There is no known cure to Alzheimer's and evidence points to the possibility of a genetic link. This study analyzes microarray data from patients with Alzheimer's disease and disease-free patients in order to evaluate and determine differential gene expression patterns between the two groups. The statistical problem stemming from this data involves many predictor variables with a small sample size, preventing the use of classical statistical approaches from being effective. We turn to a novel three-step approach: first, we screen the genes in order to keep only the genes marginally related to the outcome (presence of Alzheimer's); second, we implemented a sparse sufficient dimension reduction to retain only predictors relevant to the outcome; lastly, we perform a hierarchical clustering method to group genes that exhibit mutual dependence. We adapted this methodology from Adragni et. al and expand on their work by optimizing the existing R code with parallel capabilities in order to enhance performance speed. Thus, our results reflect both an analysis of the microarray data and a performance study of the modified code.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Meshach Hopkins was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Elias Al-Najjar was supported during Summer 2015 by UMBC.

### PROLIFERATION OF MATRIGEL-CULTURED NEURAL STEM CELLS IN VARYING OXYGEN CONCENTRATIONS

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Due to their enormous regenerative capacity, neural stem cells (NSCs) offer a potential therapeutic treatment for neurodegenerative diseases and traumatic injury. However, the extraction of embryonic stem cells from living embryos has been a controversial issue in the field of regenerative medicine. Moreover, the amount of NSCs required for treating patients immensely surpasses their availability from donors. Therefore, it is critical to develop more ethical and cost-effective methods of producing large quantities of neural stem cells. Promoting the proliferation of undifferentiated NSCs in vitro is a possible avenue for reducing the need for embryonic stem cell extraction and increasing the availability of NSCs for therapies. Oxygen plays a critical role in the viability, growth, and differentiation of NSCs in vivo. The human brain is a hypoxic environment with oxygen concentration in the range between 3-5%; however NSCs have traditionally been cultured under normoxic condition (21% O<sub>2</sub> concentration). Thus, we hypothesize that culturing NSCs under lowered O<sub>2</sub> concentration similar to the native brain tissue may increase their proliferation. To test this hypothesis, we subjected ReNcell-CX neural progenitor cells to 3% and 21% oxygen concentration for 1 day and 2 days. By running Click-iT EdU proliferation assay, we were able to detect the number of actively proliferating cells in the both hypoxic and normoxic cultures. All cells were cultured on Matrigel-coated 96-well-plates. Our results demonstrated that NSCs cultured under decreased oxygen concentration exhibit a statistically significant increase in the number of actively proliferating cells after 2 days of culture. In conclusion, proliferation of NSCs is enhanced in reduced oxygen concentrations.

This investigation was supported by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences.

## CHARACTERIZATION OF FIV MYRISTYLATED MATRIX BINDING TO MIMETIC MEMBRANES

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Feline immunodeficiency virus (FIV) is a retrovirus, similar to human immunodeficiency virus type 1 (HIV-1) in humans, that suppresses and inhibits activity of the immune system in cats. Approximately 2.5-4.4% of household cats are infected with FIV worldwide with symptoms including poor coat condition, gingivitis, diarrhea, and progressive weight loss. Studying FIV assembly is significant because humans and cats have similar immune responses, presenting a plausible target in an animal model for development of HIV-1 treatment. The Gag polyprotein consists of the following major domains: matrix (MA), capsid, and nucleocapsid. The proposed extended lipid binding model of HIV-1 depicts the interaction between MA and phosphatidylinositol-(4,5)-bisphosphate [PI $(4,5)P_2$ ], a phospholipid found in the plasma membrane; however, a limitation of this study was the use of truncated  $PI(4,5)P_2$ . The objective of this work is to use the native lipid to study its interaction with FIV MA. Liposomes, artificial lipid bilayers, are constructed that have compositions similar to that of the plasma membrane. Liposome binding assays employ nuclear magnetic resonance spectroscopy (NMR) to characterize the binding of FIV MA to PI(4,5)P<sub>2</sub> and draw comparison to interaction between HIV-1 MA and PI(4,5)P<sub>2</sub>. In addition, FIV MA has a large unstructured portion on the Cterminus that may aid in instability, so, by using mutagenesis to remove that region, it is proposed that the FIV MA stability will be increased, resulting in improved NMR data.

Howard Hughes Medical Institute, NIH/NIAID 5R37AI030917

#### ROLE OF MATRIX'S LYSINE 31 IN PROMOTING tRNA<sup>Lys3</sup> PACKAGING IN HIV-1

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Upon entry in a host cell, the HIV-1 RNA genome is reverse transcribed into double stranded DNA by reverse transcriptase using human tRNA<sup>Lys3</sup> as a primer. Packaging of virions starts with the recognition of an unspliced viral RNA by Gag and GagPol proteins, which form a complex that is targeted to the plasma membrane (PM) by the matrix (MA) domain on the Gag protein. In addition to viral machinery, cellular tRNA<sup>Lys</sup> isoacceptors are also packaged. Interestingly, the tRNA<sup>Lys3</sup> primers abundantly bind to MA in cells, this binding however, greatly decreases within the virion. It has been hypothesized that RNA binds to the Highly Basic Region (HBR) of MA, inhibiting its myristoyl group and thus enhancing MA's ability to discriminate between membranes. Since tRNA<sup>Lys3</sup> is selectively packaged, we hypothesize that tRNA<sup>Lys3</sup> binds MA during packaging and regulates MA binding to  $PI(4,5)P_2$  in the PM. We plan to characterize the structure of the MA-tRNA complex using NMR and determine the residues involved in this interaction using mutagenesis studies. Due to previous studies done on the myristate and HBR we chose to investigate further the role of Lysine 31. We used a site-directed mutagenesis approach to create the K31A mutant. We successfully purified MA HBR mutant K31A through ion exchange and size-exclusion chromatography. The binding properties of the mutant protein to tRNA<sup>Lys3</sup> will be subsequently studied through gel shift assays and isothermal titration calorimetry.

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#### DEVELOPMENT OF OPTICALLY CLEAR GLASSES FOR STUDYING IMMOBILIZED IONS, PROTEINS, AND FLUOROPHORES

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Our group worked on developing a method for studying ions, proteins, and fluorophores in an immobilized state by setting them in acrylic glass using methyl methacrylate (MMA) and poly(methyl methacrylate) (PMMA). First, different formulations were tested for creating optically clear, mechanically stable and crack-free acrylic blanks using atmospheric polymerization. Then various fluorophores were tested for solubility in liquid MMA. Those found soluble were further investigated spectroscopically for stability in the liquid monomer and the hardened polymer.

To determine the composition of the casting syrup to be used, a variety was tested. Different percentages of powdered PMMA were dissolved in liquid MMA monomer and catalyzed with 1,1'-Azobis(cyclohexanecarbonitrile), a radical initiator. Higher percentages of PMMA used resulted in a faster cure time but less optical clarity. Lower percentages of dissolved PMMA required greater cure time, but had improved optical clarity. Too much catalyst used led to crazing in the polymer's surface and too little led to a very slow reaction. A formulation of 15 % PMMA by weight, and 1 % catalyst was pursued while testing different mold materials. Mold materials tested were glass, polystyrene, polypropylene, methacrylate and RTV silicone in one and two parts. Glass performed the best, but was limiting in producing the size desired. Polystyrene and methacrylate molds reacted with the MMA and dissolved. Polypropylene and silicone molds used experienced high levels of evaporation of the casting syrup.

After the composition was resolved, fluorophores were tested for solubility in liquid MMA. Of those, eosin, NADH, NATA, perylene, POPOP, p-terphenyl, PPD, and rose bengal were further investigated for molecular stability during the polymerization process. Perylene, eosin, and POPOP showed the most stability. Those fluorophores absorbing in the ultraviolet range were masked by the absorption of the MMA monomer itself, beginning at a wavelength of around 300nm.

The authors would like to thank the Institute of Fluorescence, Department of Chemistry and Biochemistry at the University of Maryland, Baltimore County for financial support.

#### REV: THE REGULATOR OF VIRION EXPRESSION

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Human immunodeficiency virus, HIV, is a retrovirus that invades human CD4+ T cells by integrating its viral genome into the host cell's genome. Following this integration, an infected cell expresses viral accessory proteins from fully-spliced mRNA, which are exported from the nucleus via regular pathways. One such protein, Rev, facilitates a critical step in the viral replication cycle: the export of unspliced and singly-spliced viral mRNA from the nucleus to the cytoplasm. Unspliced mRNA acts as the genomic material of new virions, and also encodes for polyproteins necessary for their formation. In order to transport the mRNAs, Rev forms an oligomer on the Rev Response Element (RRE), a structural landmark located only on unspliced and singly-spliced mRNAs. The Rev-RRE complex initiates recruitment of the host's Crm1 nuclear export machinery. In order to better understand the molecular details of retroviral mRNA export, we plan to characterize the Rev-RRE interaction using a range of biophysical techniques including nuclear magnetic resonance (NMR) spectroscopy.

In order to express Rev, we used standard cloning techniques to insert the Rev gene into the pET-19b plasmid. We also introduced mutations to Rev to prevent oligomerization to aid in purification and NMR experiments. Previous studies have successfully characterized a similar construct of Rev in complex with a small portion of the RRE. However, there are few highresolution structural studies on Rev and the full RRE, primarily due to inherent difficulties in studying large RNAs. Our research aims to enhance the understanding of the interaction by forming a Rev-RRE complex with full length RRE and analyzing the interactions using NMR. Our findings will be used to elucidate the structural basis of Rev-RRE interactions to potentially guide development of therapeutics targeting this stage of the HIV-1 life cycle.

This work is supported by NIH/NIGMS grant #P50GM103297 and the Howard Hughes Medical Institute. We would like to thank Michael Summers for making our work possible and Jan Marchant for his guidance.

#### CAN ELECTRON MICROSCOPY CHARACTERIZE FLEXIBLE RNA MOLECULES?

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Electron microscopy (EM) and nuclear magnetic resonance (NMR) are powerful and complementary techniques for determining the structure of biological macromolecules, such as proteins and RNA. EM provides a global envelope structure of the molecule, but generally at lower resolution than the site-specific distance constraints provided by NMR. In contrast, NMR data is often lacking long-range information. Using these techniques in conjunction could provide a more comprehensive look at the structure of macromolecules, with the high-resolution NMR-derived structures fit to the global EM density. While these methods have been combined successfully in proteins, the flexibility of RNA renders EM more challenging for these systems. This is unfortunate, as long-range NMR constraints are particularly sparse in RNA molecules.

We will be testing the potential advantages of using multiple class averages in EM by modelling the structure of a small flexible RNA: the MMLV 5'-UTR SL-C loop. MMLV is the Moloney Murine Leukemia Virus, and the SL-C is a 43 base pair stem loop in the RNA genome. The SL-C loop has a major kink in its structure, which confers flexibility but importantly may also act as an identifying feature in determining the orientation of the individual particles in each class average. The previously characterized NMR structure will allow us to determine the best way to combine the NMR and EM data. Two constructs based on SL-C have been designed and created: SWAP, which has an altered tetraloop to prevent dimerization, and TRIM, which has some small bulges removed in addition to the altered tetraloop. We have used NMR to confirm our modifications conserve the structure of the stem-loop. Current work is focused on the preparation of samples for EM data collection and analysis.

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#### CHARACTERIZATION OF THE MONOMERIC HIV-1 RNA 5' LEADER

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Human Immunodeficiency Virus (HIV), a retrovirus which contains two copies of its RNA genome, is the causative agent of Acquired Immunodeficiency Syndrome (AIDS). HIV is a retrovirus which utilizes reverse transcriptase to reverse transcribe its RNA genome into DNA. Reverse transcriptase does not contain proofreading mechanisms, resulting in a high mutation rate. Currently, various drug therapies exist that target specific steps in HIV viral life cycle; however, finding new drug targets is vital due to the high mutation rate of the virus and noncompliance to strict drug regimens. The 5' leader (5'-L) is an untranslated region of the HIV-1 RNA genome, located at the 5' end, that controls translation and packaging through its structural conformation. The highly conserved nature of this region, unlike the rest of the genome, makes it a promising drug target. The 5'-L exists either as a monomer or dimer. The monomer is proposed to promote translation, while the dimer is selectively packaged into new viral particles.

This study utilizes nuclear magnetic resonance (NMR) techniques to characterize the monomeric structure of the 5'-L. NMR studies have allowed for confirmation of various predicted secondary structures within the monomeric 5'-L.

Because mRNA is capped *in vivo*, this study also investigates the effects of capping of the 5'-L. Native gel electrophoresis comparing the monomer-dimer equilibrium between capped and uncapped RNA show that the presence of the 5' cap stabilizes the monomeric conformation. Previous literature showed inconsistencies in the start site of the 5'-L. The current study examines the 5'-L to determine if the start site consists of one G, two Gs or three Gs.

Future studies will allow complete characterization of the secondary and tertiary structures of the 5'-L along with a further understanding of the implications of heterogeneity within the cell, regarding capping and start sites.

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#### SYNTHESIS OF WATER SOLUBLE CHLORIN

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Hydroporphyrins (chlorin and bacteriochlorin) are a promising platform for development of efficient energy transfer arrays for multicolor *in vivo* biomedical applications such as fluorescence-guided surgery (FGS) or fluorescence image-guided surgery (FIGS). Chlorins possess a strong absorption and emission in deep-red spectral window. Here we report the design, synthesis, and characterization of water-soluble chlorin, which can function as energy donor for energy transfer arrays. A 3-monobrominated chlorin with *meso*-phenyl-2,4,6-triazole polyethylene glycol chain at the 10-position (via click chemistry) was synthesized and its solubility in water was determined. The ultimate goal was to evaluate if the 2,4,6-triazole polyethylene glycol groups are responsible for the water solubilizing properties by comparing it with previously synthesized chlorins.

We anticipate that, based on previous results, the attachment of the polar motif 2,4,6triazole polyethylene glycol on the 10-position of the phenyl substituted chlorin would result in the water-solubilizing properties of this chlorin as compared to previously synthesized chlorins bearing only the triethylene glycol (TEG) chain. Upon achieving this goal we would like to incorporate the resulting chlorin into a multi-system architecture bearing the chlorinbacteriochlorin array linked by an amide functionality that can be used for *in vivo* multicolor imaging.

This investigation was supported in part by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences, and NCI-NIH under award U01CA181628.

#### NON-IMAGE FORMING VISUAL PIGMENTS: DO THEY INTERNALIZE?

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G protein-coupled receptors (GPCRs), the largest family of eukaryote transmembrane receptors, respond to extracellular stimuli and trigger a response within the cell. Opsins are specialized GPCRs that are involved in the conversion of light into a biological signal. Melanopsin is an opsin that is found in intrinsically photosensitive retinal ganglion cells (ipRGCs) in the mammalian retina and regulates non-image forming functions such as circadian photoentrainment and pupillary constriction. While much of the phototransduction pathway of melanopsin remains unknown, we hypothesize that melanopsin is internalized after activation by light and deactivation by  $\beta$ -arrestin. To test this hypothesis, we synthesized GFP-tagged melanopsin constructs in a mammalian expression vector, PMT3, through cassette mutagenesis and expressed these constructs in Human Embryonic Kidney (HEK293) cells. We then compared localization of melanopsin is internalized in a heterologous expression system.

This work was funded by NSF DBI-1031420.

# SUCCESSFUL NAVIGATION WITH THE INTEGRATION OF ARCHITECTURE AND ORIENTATION AND MOBILITY TRAINING USED BY VISUALLY IMPAIRED ADULTS

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Independent navigation when an individual is visually impaired can be difficult at first, but with practice and training, the journey to the destination becomes a much easier task. Environmental information is effective in determining the successful outcome of independent navigation, but blind individuals must also rely on their previous training in orientation and mobility in addition to environmental cues in order to reach their destination. The purpose of this research is to examine how certain architectural features are used with blind navigators' previous training in orientation and mobility to successfully reach their destination. We conducted focus group studies and first-hand observations composed of adults with vision impairments from Washington DC and Atlanta, Georgia. Open data coding was used to find common themes from their statements, with a strong focus of their usage of their training alongside architectural structures which resulted in successful navigation. These studies revealed that certain architectural features including unique structures such as fountains, texture changes on the ground, and audible crosswalks were useful while navigating. By creating "mental maps" while traveling with the addition of these architectural features, blind navigators can easily determine where they are spatially in relation to streets and buildings. By using the research findings of this study, further education of the public on how blind people navigate could be especially useful in the future development of technology and architecture which would allow more accessibility of routes and destinations to both blind and sighted navigators alike.

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#### OVEREXPRESSION OF NAR1.2 AND LCI1 IN CHLAMYDOMONAS REINHARDTII

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Grown under optimal conditions algae have the ability to use free resources ( $CO_2$  and sunlight) to grow rapidly as well as produce significant amounts of biomass that can be converted into biofuel to be used as an alternative to fossil fuels. The aim of this project is to improve the growth rate of *Chlamydomonas reinhardtii*. This green alga is a model organism for lab research because its whole nuclear genome is known, and many molecular genetic tools make it easy to manipulate. We are focusing our efforts on the carbon concentrating mechanism (CCM), which regulates CO2 uptake in the organism, and more specifically on two  $CO_2$ transporters, LCI1 and NAR1.2. LCI1 (low CO<sub>2</sub> induced) localizes in the plasma membrane and NAR 1.2 functions in the chloroplast envelope. Our overall goal is to overexpress these proteins by ligating the coding sequences for the LCI1 and NAR1.2 genes into C. reinhardtii nuclear expression vector pARG and then transforming into C.reinhardtii. Thus far we have succeeded in generating the expression vectors for both LCI1 and NAR1.2, and have obtained transformants for the NAR1.2 vector. Multiple lines of the transformed algae were cultured and are being tested by western blot analysis. We will do growth curve and biomass accumulation analyses on the best expressing strains. If we are successful in improving algal growth by overexpressing NAR1.2 and/or LCI1, the next step will be to express these enzymes in the Chlorella vulgaris, a green alga that is related to C. reinhardtii but a much better commercial production organism.

The results were obtained as part of the Research Experience and Mentoring (REM) program in the Department of Biological Sciences at the University of Maryland Baltimore County. The program is funded by a grant (REM supplement to NSF-EFRI-1332344) from the National Science Foundation (NSF) Directorate for Engineering (ENG) Office of Emerging Frontiers in Research and Innovation (EFRI).

# EFFECTS OF A CHROMATIN REMODELER ON MIGRATORY CELL FATE DETERMINATION

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Cell migration is a critical process in the normal development and functioning of organisms in capacities such as wound healing, tissue formation, and immune response. To understand better the mechanisms that determine cells to be migratory or static, we examine collective cell migration in the ovarian tissue of the organism *Drosophila melanogaster*. During egg development in Drosophila, a small subset of somatic epithelial cells are specified as "border cells" which form a cluster and migrate from the anterior pole of the egg chamber toward the oocyte. The highly conserved Janus Kinase/Signal Transducer Activator of Transcription pathway (JAK/STAT) regulates this process, and two downstream targets of the transcription factor STAT, *apontic (apt)* and *slow border cells (slbo)*, are crucial in determining border cell fate.

Previous work has shown that Brahma, a chromatin remodeler affecting availability of DNA for transcription, has an effect on border cell migration through interaction with the JAK/STAT cascade, but its role is still unclear. To investigate Brahma's function, we conducted a series of genetic experiments comparing the migratory phenotypes of *brahma* mutants to controls. Further, to discover genetic interactions between *brahma* and *apt* or *slbo*, we utilized RNA interference (RNAi) to knockdown Brahma in conjunction with each of them and observed the effect on cluster migration.

To simulate Brahma's role in this genetic circuit mathematically, we used an existing model of differential equations representing this pathway that reflects the static versus motile bistability of the system. Into this we introduced a parameter for Brahma, and through bifurcation analysis and a numerical simulation, have shown the effect of Brahma on the system under the assumptions indicated by our experimental results. This work should help further understanding of the impact of chromatin remodeling on the pathways regulating collective cell migration across organisms at large.

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#### EXPLORATION OF ATOMIC FORCE MICRSCOPY (AFM)

#### <u>Chloe A. Kwon</u>, Margaret E. LaCourse, Ian W. Shaffer, Joshua A. Wilhide, William R. LaCourse Molecular Characterization and Analysis Complex (MCAC), UMBC 1000 Hilltop Circle, Baltimore MD 21250

Evolution of microscopy over the years has greatly improved imaging. In particular, 1986 marked the start for a method of microscopy known as atomic force microscopy (AFM). Containing a probe with a tip radius of around 300nm at the end that is responsible for scanning the surface of the sample, AFM allows users a wider range of applications with minimal sample preparation. A laser beam is deflected off the tip onto a photodiode, which measures the specific mechanical movements of the probe to produce an image of the sample. AFM offers three modes of operation (i.e., tapping, contact, and non-contact) to maximize the options of applications. For instance, AFM is capable of imaging proteins, blood cells, bacteria, viruses, polymers, metals, and minerals.

The MCAC houses an Axiovert 100 BioScope II. Since this instrument has not been heavily used for many years and has no current experienced user, the goal of this research is to become more familiar with a technique that allows proper calibration and engagement of the microscope using a NCHV-A silicon probe. Future applications for the AFM include analyzing a variety of atomic level structures to test the capabilities and parameters of the instrument. This research will be an on-going project to image additional samples and continue learning the proper methods and preparation involved with atomic force microscopy.

On behalf of the MCAC, I would like to thank Bruker for their assistance with instrumentation and troubleshooting. Furthermore, I would like to personally thank the members of the MCAC for allowing me the opportunity to utilize their facility and instruments to further my understanding and experience as an undergraduate researcher.

THE ROLE OF CALCIUM IN METABOLIC OSCILLATIONS OF PANCREATIC BETA CELLS REU Site: Interdisciplinary Program in High Performance Computing <u>George Eskandar<sup>1</sup>, Jennifer Houser<sup>2</sup>, Ellen Prochaska<sup>3</sup>, Jessica Wojtkiewicz<sup>4</sup>,</u> Graduate assistant: Teresa Lebair<sup>5</sup>, Faculty mentor: Bradford E. Peercy<sup>5</sup>, Clients: Margaret Watts<sup>6</sup> and Arthur Sherman<sup>6</sup> <sup>1</sup>Department of Computer Science and Electrical Engineering, UMBC <sup>2</sup>Department of Mathematics, East Tennessee State University <sup>3</sup>Department of Mathematics, Creighton University <sup>4</sup>Department of Mathematics, Louisiana State University <sup>5</sup>Department of Mathematics and Statistics, UMBC <sup>6</sup>Laboratory of Biological Modeling, National Institutes of Health

In order to further understand diabetes mellitus, it is necessary to investigate the dynamics of insulin secretion in the bloodstream. Diabetes is a disease characterized by improper concentrations of blood glucose due to irregular insulin production. Beta cells are responsible for the production and regulation of insulin based on changes in glucose levels. Clusters of these cells, known as islets of Langerhans, are part of the endocrine system in the pancreas. Ultimately, insulin secretion occurs because of changes in the calcium concentration levels in beta cells. This dynamical process is composed of electrical, metabolic, and mitochondrial components that work together to release insulin into the blood. A mathematical model has been developed that captures the full dynamics of insulin secretion including the fast- and slow-bursting behavior from electrical and glycolytic oscillations, respectively.

Using the Dual Oscillator Model, we will examine how calcium handling within individual pancreatic beta cells affects the synchronization of metabolic oscillations within electrically coupled islets. Calcium permeability was implemented into the Dual Oscillator Model, and numerical solutions of the system were obtained via Matlab using a modified ordinary differential equation solver for stiff systems and the Automatic Differentiation for Matlab software. A synchronization index has been developed to quantitatively describe the synchronization of variables between nearest neighboring cells and throughout the islet as a whole. We consider how calcium diffusion between heterogeneous cells affects the behavior of metabolic oscillations and their synchronization. In particular, we want to examine fructose-1, 6bisphosphate and glucose-6-phosphate. Our research will show whether calcium diffusion between cells enhances, diminishes, or terminates metabolic oscillations.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author George Eskandar was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Teresa Lebair was supported during Summer 2015 by UMBC.

#### DETERMINING THE STRUCTURE OF THE REV RESPONSE ELEMENT IN HIV-1

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The Rev Response Element (RRE) is a noncoding portion of the HIV-1 genome found on unspliced and singly-spliced transcripts. The accessory protein Rev interacts with the RRE, facilitating nuclear export of these RNAs. Our research focuses on solving the secondary, and eventually tertiary, structure of the RRE using nuclear magnetic resonance (NMR).

Large RNAs such as the RRE (233 nucleotides) are particularly difficult to analyze by NMR due to broad signals and overlapping peaks. The strategy we used to overcome this challenge involved making smaller fragments based on various computational predictions of the full length RRE secondary structure. The comparison of the fragments and full-length spectra can inform us on the presence or absence of these fragments in the structure. With this strategy, we detected a number of elements consistent with the lowest energy secondary structure prediction. To investigate more complicated regions of the RRE, we designed a segmentation strategy in which we split the RRE at one of our confirmed stem loops, which was replaced by complementary base pairs. By independently transcribing these segments, different labeling schemes can be applied to each before they are annealed back together. These differentially-labeled samples assist with the assignment of chemical shifts and distance constraints by enabling precise editing of our NMR spectra.

We will use these assignments to aid further characterization of the RRE structure, providing insight into the details of retroviral RNA nuclear export, thus potentially advancing the development of therapeutics targeting this stage of the HIV-1 life cycle.

We would like to acknowledge the NIH/NIGMS #P50GM103297, as well as the Howard Hughes Medical Institute and Dr. Summers for the opportunity to participate in advancing scientific research.

#### GENETIC SCREENING OF RGMA MUTANTS

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Repulsive Guidance Molecule family member a (Rgma) is a GPI-anchored membrane protein that inhibits regeneration and assists differentiation. In order to explore Rgma function in the developing central nervous system (CNS), we mutagenized Exon 2 and 3 of the *Rgma* locus in zebrafish embryos using the universal CRISPR/Cas9 system. Manipulated founders (F0s) were screened by PCR, restriction digest, and high resolution melting analysis (HRMA) and had a mutation rate of ~80%. However, F0 tissues are mosaic for wild type (WT) or various mutant *Rgma* alleles. Stable mutant alleles were isolated by generating heterozygous F1 progeny produced by a F0 X WT cross and screening larvae or adult tissues using the above methods. We will use our CRISPR mutants to investigate the role of *Rgma* during neural convergent extension (NCE), an early, conserved stage of neural tube development that is marked by high Rgma expression. We predict that our targeted mutagenesis approach will overcome the specificity challenges of Morpholino (MO) work.

I would like to thank Julie Wolf, Pradeepa Jayachandran, Austin Gabel and Neus Sanchez Alberola.

#### ASSESSING DECADAL CLIMATE IMPACTS ON WATER RESOURCES WITHIN MISSOURI RIVER SUB-BASINS

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It is well documented that decadal climate variability (DCV) has a significant impact on water resources in the Missouri River Basin (MRB). This project aims to utilize multi-decadal simulations of Global Climate Models (GCM) from the Climate Model Inter-comparison Project (CMIP5) to assess the DCV impact on water yield and streamflow over the MRB using a widely utilized hydrology and crop model known as the Soil and Water Assessment Tool (SWAT).

We use low-resolution (~100km x 100km) data from MIROC5 and HadCM3 GCMs with 57 years of climate simulations at approximately 30,000 locations. The weather parameters included in the GCMs are monthly precipitation, maximum/minimum temperatures, sea-level pressure, relative humidity, and surface wind speed. We downscale all the parameters to match high resolution (12km x 12km) observed data using a two-step procedure. First, an interpolation method is utilized to fill in values at locations where the weather parameters are not available, and then multiple linear regression (MLR) is used to capture features of the observed data at the higher resolution. The coefficients from regression are combined with hindcast data from the two GCMs to compute monthly predictions of maximum/minimum temperatures, and precipitation to input into SWAT. A Weather Generator tool in SWAT is used to generate the daily values necessary to input into SWAT from predictions and observed weather statistics.

We modified a previously developed Graphical User Interface (GUI) in R to streamline the process and include more options for users. We explore if the use of different GCMs and the addition of MLR improves the accuracy of predicting the above-mentioned variables in the MRB. The procedures and GUI developed in this project will allow the client to conduct numerous studies with improved efficiency to assess sensitivity of water resources within the MRB resulting from climate variability and change scenarios.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Per- formance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS–0821258 and CNS– 1228778) and the SCREMS program (grant no. DMS–0821311), with additional substantial support from UMBC. Co-author Kwame Owusu-Boaitey was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Sai K. Popuri was supported during Summer 2015 by UMBC.

#### THE LARGE SCALE SYNTHESIS AND EXTRACTION OF RIBONUCLEIC ACIDS

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Ribonucleic acids (RNA) play a variety of roles in cellular function and are critical to the regulation of genetic information, catalysis of chemical reactions, and crucial in protein translation. In pursuance of a better understanding of the structure and function of RNAs, they must first be synthesized and extracted through a multi-step process. The process utilizes various laboratory techniques through which RNA is transcribed in vitro, and then purified for study. RNA is transcribed from recombinant DNA, which is isolated from bacterial cells using the QIAGEN MegaPrep kit. This newly isolated DNA template is then used in a small scale trial transcription reaction, which is designed to optimize conditions and maximize RNA yield in the large scale reaction. RNA is isolated from the large scale reaction through gel electrophoresis, and then extracted and purified. This newly purified RNA can then be utilized for in vitro biophysical, structural, and biochemical study - an application of which is in the structural characterization of the 5'-Untranslated Region (5'-UTR) in the HIV-1 RNA genome.

This research was funded by NIH/NIGMS grant *1P50GM103297*, and was conducted at the Howard Hughes Medical Institute at UMBC with support in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. We would also like to thank our research team Seungho Choi<sup>2</sup>, Eric Cormack<sup>3</sup>, Hannah Carter<sup>2</sup>, and Aishwarya Iyer<sup>2</sup> for their assistance.

#### MICROWAVE LYSING AND FRAGMENTATION OF LISTERIA

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The isolation of DNA from bacterial cells has historically been a time-consuming and expensive process. Given the usefulness of microwaves in heating biological systems, a microwave-based process for the isolation of DNA has proven beneficial in terms of cost and speed. Here we describe approaches for the rapid isolation of DNA using a traditional microwave. The use of geometric gold triangles can assist to focus microwaves and thus lyse the bacterial cells and fragment the released DNA. The long term goal of this project is to lyse, fragment, and detect listeria using a rapid and sensitive method known as Microwave-Accelerated Metal-Enhanced Fluorescence (MAMEF). MAMEF is a faster and cheaper method for the detection of microbial pathogens than traditional molecular methods such as polymerase chain reaction (PCR).

#### UNDERSTANDING COMMENTING IN VLOGGING COMMUNITIES

Imani McLaurin<sup>1</sup>, Wayne Lutters<sup>2</sup>, Stacy Branham<sup>2</sup> <sup>1</sup>Department of Computer Science, Bowie State University, 14000 Jericho Park Rd, Bowie, MD 20715 <sup>2</sup>College of Engineering and Information Technology, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Online access of this abstract is restricted at the request of the Principal Investigator.

## CRYSTALLIZATION OF THE RIBONUCLEOPROTEIN COMPLEX THAT NUCLEATES VIRAL ASSEMBLY

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Human immunodeficiency virus (HIV) is a retrovirus that is responsible for about two million deaths globally each year. Although treatment regimens target various phases of the viral life cycle, increasing instances of drug resistance require the development of new drugs and identification of new drug targets. Viral RNA elements residing in the conserved 5' leader of the HIV-1 genome direct packaging and are recognized by the nucleocapsid (NC) domains of the viral Gag polyprotein. Previous work from our lab identified a 155-nucleotide region in the 5' leader, the Core Encapsidation Signal ( $\Psi^{CES}$ ) that directs genome recognition and packaging. Our goal is to determine the tertiary structure of the  $\Psi^{CES}$  and NC-bound  $\Psi^{CES}$  complex through X-ray diffraction.

The structural flexibility and conformational heterogeneity of  $\Psi^{CES}$  is a potential impediment to obtaining suitable crystals for X-ray diffraction studies. Therefore, two approaches aimed at stabilizing the structure of  $\Psi^{CES}$  were applied. First, a pair of mismatched stacked pyrimidines in the native  $\Psi^{CES}$  serves as a flexible hinge for the extended Dimerization Initiation Site (DIS) hairpin. A canonical pair of mutations was introduced at that site to reduce flexibility of the DIS arm. Second,  $\Psi^{CES}$  binds eight NC proteins with high affinity. NC binding to  $\Psi^{CES}$  may increase the likelihood of crystallization by reducing flexibility. Native and mutated  $\Psi^{CES}$  constructs will each be crystallized with and without NC proteins. The X-ray diffractionderived tertiary structure of the  $\Psi^{CES}$ , particularly in complex with NC, will be crucial in understanding the molecular function and mechanism of HIV-1 genome recognition and packaging, driving the development of targeted therapies.

This research was funded by NIH/NIGMS grant 1P50GM103297 and was conducted at the Howard Hughes Medical Institute at UMBC, with support from the Summer Biomedical Training Program (SBTP). Supported in part by the Howard Hughes Medical Institute's Summer Medical Fellows, Precollege and Undergraduate Science Education Programs. We would also like to thank our research team: Gregory Carter, Alyssa Florwick, Justin Santos, Heather Frank, Briaunna Minor, and Carly Sciandra for their assistance.

#### OVEREXPRESSION OF CAH1 AND CAH8 IN CHLAMYDOMONAS REINHARDTII

Binika Chunara<sup>1</sup>, Nicholas Often<sup>1</sup>, Rose Gbemafu<sup>1</sup>, Rudolph Park<sup>2</sup>, Amrita Madabushi<sup>1</sup>, and Stephen M. Miller<sup>2</sup> <sup>1</sup>BCCC, 2901 Liberty Heights Avenue, Baltimore, MD 21215 <sup>2</sup>Department of Biological Sciences, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Lipids derived from algae hold great promise as a sustainable fuel source. However, commercial production of algal fuels is expensive in comparison with fossil fuel. Genetic manipulation of algae can make biofuel production more efficient. The photosynthetic green alga Chlamydomonas reinhardtii is a well-studied model organism that is easily manipulated at the molecular genetic level. In this study we are focusing on improving the carbon concentrating mechanism (CCM), a biological adaption to low carbon dioxide levels in the atmosphere. The CCM is composed of mainly three components: carbonic anhydrases, CO<sub>2</sub> transport proteins, and the pyrenoid. Carbonic anhydrases catalyze the interconversion of carbon dioxide and bicarbonate and thereby make inorganic carbon more accessible to the cell. The aim of this study is to increase the uptake of CO<sub>2</sub> in C. reinhardtii by overexpressing two periplasmic (between the cell wall and membrane) carbonic anhydrases, CAH1 and CAH8, and ultimately determining the effect on growth rate. C. reinhardtii CAH1 and CAH8 coding regions were synthesized with C. reinhardtii codon bias and epitope tags and the gene fragments were subcloned into expression vector pARG which contains the ARG7 gene required for arginine biosynthesis. We transformed the CAH1 vector into an arg7 mutant strain and selected several ARG<sup>+</sup> survivors for western blot analysis to determine the expression of protein; CAH8 lines will be generated later. We will select the best expressing lines for growth curve and dry weight analysis to determine whether the transformants overexpressing CAH1 or CAH8 are able to grow faster than the wildtype C. reinhardtii strain. In future both genes could be expressed together. If we are successful, the next step will be to incorporate these methods for microalgae that naturally produce higher lipid levels than C. reinhardtii, but are harder to manipulate, such as Chlorella vulgaris.

These results were obtained as part of the Research Experience and Mentoring (REM) program in the Department of Biological Sciences at the University of Maryland Baltimore County. This program is funded by a grant (REM supplement to NSF-EFRI-1332344) from the National Science Foundation (NSF) Directorate for Engineering (ENG) Office of Emerging Frontiers in Research and Innovation (EFRI).

#### CHARACTERIZATION OF THE HIV-1 5' UTR DIMERIZATION MECHANISM

#### Justin Leonel C. Santos, Carly A. Sciandra, Sarah C. Keane, and Michael F. Summers Department of Chemistry and Biochemistry, Howard Hughes Medical Institute, UMBC, 1000 Hilltop Circle, Baltimore, MD 21052

Human immunodeficiency virus type-1 (HIV-1) is responsible for a pandemic that affects roughly 35 million people worldwide. There is no known cure and antiretroviral medications only serve to reduce the progression of the disease. Current treatments target four stages of the viral life cycle: entry, reverse transcription, integration, and maturation. There is currently no treatment that targets the genome recognition and packaging phase of the viral life cycle. HIV-1 selectively packages the dimeric, unspliced RNA genome. Our group is attempting to understand the structural mechanism behind HIV-1 packaging selectivity. Evidence shows that dimerization of the HIV-1 genome is initiated by a palindromic GCGCGC sequence at the Dimerization Initiation Site (DIS) in the 5' leader (5'-L) between two strands of unspliced RNA. However, previous studies in our lab have shown that the 5' L dimer exhibits a more extensive intermolecular interface. We will employ NMR spectroscopy using a mutagenesis strategy known as long-range probing by Adenosine Interaction Detection (lr-AID) in order to further characterize this mechanism as a function of time. RNA samples will be prepared with specific deuterium labeling in order to probe the dimer conformation at different time intervals. At short time intervals we hypothesize that the HIV-1 5'-L dimerization to transition from a "kissing" loop interaction into a more extensive intermolecular dimer interface. Furthermore, we aim to utilize these results into the development of new therapies that target genome selection for packaging.

This research was funded by NIH/NIGMS grant *1P50GM103297* and NIGMS MARC USTAR grant *T34GM00866*, and was conducted at the Howard Hughes Medical Institute at UMBC with support from the Summer Biomedical Training Program (SBTP). Supported in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. We would also like to thank our research team Gregory Carter, Alyssa Florwick, Briaunna Minor, Heather Frank, Dianne Omire-Mayor, and Mian Khalid for their assistance.

# THE IMPACT OF MYELOID-DERIVED SUPPRESSOR CELLS ON OBESITY AND ITS ASSOCIATION WITH CANCER

#### Ramses Long, Tiha Long

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Obesity is a known risk factor for developing cancer and is accompanied by an increase in Myeloid-derived suppressor cells (MDSC). MDSC are immune suppressive cells that accumulate during tumor progression and inhibit the immune system from eliminating cancer. Because of the association of obesity, MDSC, and cancer, we are investigating whether MDSC merely correlate with obesity or contribute to obesity and the obesity-induced cancer risk (or vice-versa). To determine the role of MDSC in obesity we will induce or deplete MDSC in mice on a high fat diet (HFD) to promote obesity or a low fat diet (LFD) as a control for dietassociated changes. We will measure changes in insulin, glucose, inflammation and weight gain in each group. We hypothesize that induction of MDSC in mice on the HFD will demonstrate the greatest increase in weight, decreased insulin resistance, increased glucose tolerance and reduced inflammation, compared to controls. To test this hypothesis, we are developing a protocol to maintain elevated levels of circulating MDSC by inoculating mice with granulocyte colony stimulating factor (G-CSF), a cytokine that induces MDSC proliferation by binding to G-CSF receptor (G-CSF-R) on MDSC. Mice inoculated with 1000 or 500 µg/kg G-CSF have 37% and 33% circulating MDSC, respectively, as compared to untreated mice, which have 8-16% MDSC. Previous studies demonstrated these doses increase MDSC levels. On-going studies are determining the efficacy of lower doses of G-CSF (e.g. 250 µg/kg). To determine the kinetics of G-CSF-R expression we used flow cytometry to measure G-CSF-R post-injection. Receptor levels decreased following G-CSF injection, but returned to basal levels 2-3 days after 500 or 1000 µg/kg doses, respectively. We are determining the optimal dosing schedule for sustaining G-CSF-R while elevating circulating MDSC so we can evaluate MDSC impact on metabolic functions in obesity and the associated increase in cancer risk.

#### PROTEIN: RNA INTERACTIONS THAT NUCLEATE HIV-1 VIRAL ASSEMBLY

<u>Heather Frank<sup>1</sup>, Briaunna Minor<sup>2</sup></u>, Sarah C. Keane<sup>1</sup>, and Michael F. Summers<sup>1</sup> <sup>1</sup>Department of Chemistry and Biochemistry, Howard Hughes Medical Institute at UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>2</sup>Department of Biology, Xavier University of Louisiana, 1 Drexel Drive, New Orleans, LA 70125

36 million people are currently infected with human immunodeficiency virus (HIV), a retrovirus responsible for the onset of the acquired immunodeficiency syndrome (AIDS). Upon transmission, the virus invades CD4<sup>+</sup> T cells and integrates its proviral genetic material into the host genome leading to a life-long infection. During the viral life cycle, interactions between the unspliced viral RNA and its translated product, the Gag polyprotein, initiate the packaging of two copies of the HIV genome. Gag contains three structured domains: Matrix (MA), Capsid (CA), and Nucleocapsid (NC). The NC domain of Gag binds to regions of the 5'-leader (5'-L) within the dimeric HIV-1 genome to initiate genome packaging and viral assembly.

We seek to characterize the Gag-RNA interactions essential to genome packaging through the use of both mature NC and a truncated Gag derivative, CA-p2-NC (CANC). Capsidcapsid interactions promote the formation of distinct units called hexamers. We hypothesize that the hexameric structure of the CA domain contributes to dimeric RNA genome selection. However, hexamer-hexamer interactions in the C-terminal Domain (CTD) of CA lead to protein aggregation and precipitation in the presence of RNA. To circumvent these problems we have introduced W184A and M185A mutations into the CTD of the CA domain of CANC. These mutations prevent the CTD interactions that cause dimerization among hexamers. With these three protein constructs, we aim to deduce the qualitative conditions and thermodynamic parameters of these Gag-RNA interactions using electrophoretic mobility shift assays (EMSA) and isothermal titration calorimetry (ITC).

This research was funded by NIH/NIGMS grants *1P50GM103297* and *8665942* and was conducted at the Howard Hughes Medical Institute at UMBC, with support from the Summer Biomedical Training Program (SBTP) and by the NIH-funded MARC U-STAR Program at Xavier University of Lousiana. In addition, we'd like to thank members of our research team – G. Campbell Carter, Alyssa T. Florwick, and Justin Leonel C. Santos, Carly Sciandra, Mian Khalid and DianneMarie Omire-Mayor.

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# Poster Session 2

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Hollie	Adejumo	Independent Research	88
Amanda	Alexander	HPC REU	16*
Chuk	Amaefule	Independent Research	64
Ely	Biggse	HPC REU	8*
Tiana	Boardley	MARC U*STAR Trainee	24
Margarita	Brovkina	Independent Research	50
Grace	Canham	SBTP Trainee	82*
Paige	Canova	Independent Research	56*
Haneet	Chadha	MARC U*STAR Trainee	46
Wesley	Collins	HPC REU NSA Scholar	22*
Jordan	Damon	Independent Research	100
Braxton	Dubin	Independent Research	72
Joseph	Emelike	HPC REU	86*
Heather	Frank	Independent Research	102*
Eric	Frazier	HPC REU	16*
Malique	Georges	SBTP Trainee	60
Charles	Gray	SBTP Trainee	42
Tarik	Hawkins	MARC U*STAR Trainee	32*
Meshach	Hopkins	HPC REU	52*
Jennifer	Houser	HPC REU	80*
Oluwagbotemi	Igbaroola	MARC U*STAR Trainee	92
Samuel	Keating	Independent Research	2
Mian	Khalid	Other	94*
Tahsin	Khan	UBM	70*
Megha	Kori	Independent Research	68
Rushmie	Kulkarni	UBM	4*
Alex	Kuznetsov	Other	38*
Daniel	Martinez	DREU	18*
Michael	McCauley	HPC REU	16*
Travis	McKay	HHMI Scholar	20
Lindsay	Mercer	UBM	76*
Lauryn	Mitchell	HHMI Scholar	78
Chang-Wu	Mungai	SBTP Trainee	66*
Pranesh	Navarathna	Independent Research	74
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# Poster Session 2 (Continued)

First Name	Last Name	Program Affiliation	Poster #
Brandon	Osborne	HPC REU	48*
Kwame	Owusu-Boaitey	HPC REU	86*
Sarah	Pollock	MARC U*STAR Trainee	10
Ellen	Prochaska	HPC REU	80*
Rebecca	Rachan	HPC REU	52*
Rebekah	Rashford	HHMI Scholar	6
Amalia	Rivera-Oven	Independent Research	58*
Glorianne	Rivera-Santiago	JCET	40
Julio	Roman	JCET	34*
Graham	Rubin	Independent Research	36
Beatrice	Rukenwa	Independent Research	96
Gabrielle	Salib	HPC REU	48*
		HHMI Scholar	00*
Justin	Santos	MARC U*STAR Trainee	98.
Christian	Sias	JCET	84
Amelia	Smith	Independent Research	54
Roald	Teuben	Other	62*
Kechera	Tilghman	SBTP Trainee	44*
Jonathan	Werner	Independent Research	12*
Chantel	Wilson	HHMI Scholar	30
Abenezer	Wudenhe	HPC REU	28*
Elangeni	Yabba	SBTP Trainee	26
Jessica	Zaki	Independent Research	14
## COPPER TOXICITY AND REMEDIATION IN E. COLI: A DYNAMIC MATHEMATICAL MODEL

<u>Samuel Keating</u><sup>1</sup>, Dr. Bradford E. Peercy<sup>2</sup> <sup>1</sup>Department of Chemical, Biochemical, and Environmental Engineering, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>2</sup>Department of Mathematics and Statistics, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Copper is an element that is essential in small amounts, but can be toxic in large concentrations. Many methods have been used to reduce the amount of copper in polluted water. The most effective of these methods involve the use of bacteria trained to resist copper's toxicity. I am in the process of constructing a mathematical model to track bacterial cells' ability to withstand and remove toxic levels of copper in polluted waters. This model is constructed using Michaelis Menten kinetics for the enzymatic reactions occurring inside the cell, tracking the uptake rate of copper from the water into the cells, and running an ordinary differential equation solver in MATLAB to find the dynamic relationships between the different chemical species over time. These resulting computations are used to account for the number of cells that are killed by the toxic reactive oxygen species that copper is a catalyst for. This project has applications in genetic engineering and can take inputs for varying concentrations of copper enzymes to model the effects of upregulating genes for these enzymes. By analyzing the outputs of this model, an optimum concentration of these enzymes can be found that maximizes copper uptake while minimizing cell death.

I have constructed a MATLAB Graphical User Interface (GUI) that plots the dynamic behavior of this system over time with changing inputs. The GUI plots the concentrations of 9 out of the 14 chemical species tracked by this model. The GUI allows for varying concentrations of the copper enzymes superoxide dismutase, catalase, and metallothionein and plots the resulting chemical concentrations inside the cell and the percent of cells that are dead.

I would like to acknowledge the UMBC iGEM Team, the UMBC Student Government Association, the UMBC College of Natural and Mathematical Sciences, UMBC Biology Department and UMBC Chemistry Department for their financial support without which this project would not be feasible.

## GENE EXPRESSION NETWORKS OF HISTONE METHYLTRANSFERASES SET1 AND SET5 IN S. CEREVISIAE

<u>Grace H. Choi</u><sup>1\*</sup>, <u>Rushmie Kulkarni</u><sup>2\*,</sup> DoHwan Park<sup>1</sup>, Erin Green<sup>2</sup> <sup>1</sup>Department of Mathematics & Statistics, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>2</sup>Department of Biological Sciences, UMBC, 1000 Hilltop Circle Baltimore, MD 21250 \* These authors contributed equally to this work

Histone methyltransferases Set1 and Set5 play key roles in the modification of chromatin to regulate gene expression. In 2014, Martin et al. characterized new functional consequences of losing either one or both Set1 and Set5 in budding yeast. This work revealed that both methyltransferases are important for repressing lowly expressed genes near telomeres and retrotransposons. Our study revisits this raw data and performs alternative methods of RNA-seq analysis for gene expression profiling under a Bioconductor/R pipeline and CLC Genomics workbench protocol. After determining significant differentially expressed genes compared to a wild type (WT) strain, we performed hierarchical clustering and correlation analysis between the set 1 $\Delta$ , set 5 $\Delta$ , and set 1 $\Delta$  set 5 $\Delta$  mutants and microarray data of 16 additional strains lacking wellknown chromatin regulators. Clustering based on a Pearson's correlation distance matrix indicates Set5 has an overlapping role with the histone deacetylase Rpd3 and Set1 works in tandem with COMPASS complex components. Preliminary gene ontology (GO) analysis shows significant enrichment for genes involved in sporulation in the set  $1\Delta$  and set  $1\Delta$  set  $5\Delta$  datasets, suggesting an additional function of these histone methyltransferases. Overall, this method of RNA-seq analysis expands our understanding of Set1 and Set5's function and pathway relationships in the regulation of gene expression.

This work was funded, in part, through an Undergraduate Biology Mathematics (UBM) Award from the National Science Foundation under Grant No. DBI 103140, PIs Drs. Leips and Neerchal.

#### RIBOSOMAL PROTEIN L4 BINDING DURING RIBOSOMAL RNA MATURATION

<u>Rebekah Rashford</u>, Jesse Fox, Lasse Lindahl Department of Biological Sciences, UMBC, 1000 Hilltop Circle, Baltimore, Maryland 20879

Ribosomal RNA (rRNA) and ribosomal proteins are integral parts of the ribosome complex found in all organisms. These particles undergo an extensive synthesis process in which rRNA and ribosomal proteins join together to from mature ribosomes. Much research has been conducted to determine the structure of mature ribosomes (through x-ray crystallography) and the maturation process of rRNA, but at which point the ribosomal proteins join the pre rRNAs is still yet to be better understood.

Using the large subunit (60S) ribosomal protein L4 as the protein of interest, we studied when during the maturation process of rRNA did L4 bind to one of the pre-rRNAs. By utilizing and optimizing co-immunoprecipitation assays specific for the nine amino acid hemagglutinin (HA) protein tag, we were able to target the point at which HA-L4 binds to the pre-rRNA.

Using northern blot analysis and DNA probes specific for the latest pre-60S rRNAs, we found that L4 binds to the 27S and 7S pre-rRNA segments, meaning that L4 binds prior to the C2 cleavage site being cut. The next step is to use different probes on L4 to determine whether L4 is found at earlier cleavage sites (such as A2 or A3). Using this information, we will be able to indicate L4s first encounter with pre-rRNA during the maturation process.

This research was supported in part by a grant to UMBC from the Howard Hughes Medical Institute through the Precollege and Undergraduate Science Education Program.

## NUMERICAL EVALUATION OF MINIMUM AVERAGE DEVIANCE ESTIMATION IN ULTRA HIGH DIMENSIONAL POISSON REGRESSION

REU Site: Interdisciplinary Program in High Performance Computing <u>Ely Biggs</u><sup>1</sup>, <u>Tessa Helble</u><sup>2</sup>, <u>George Jeffreys</u><sup>3</sup>, <u>Amit Nayak</u><sup>4</sup>, Graduate assistant: Elias Al-Najjar<sup>2</sup>, Faculty mentor: Kofi P. Adragni<sup>2</sup>, Client: Andrew Raim<sup>5</sup> <sup>1</sup>Department of Applied Mathematics, Wentworth Institute of Technology <sup>2</sup>Department of Mathematics and Statistics, UMBC <sup>3</sup>Department of Mathematics, George Washington University <sup>4</sup>Department of Mathematics, George Washington University <sup>5</sup>US Census Bureau

The second most expensive part of US Census Bureau's decennial census in 2010 was Address Canvassing (AdCan), a door-to-door data collection in order to update the Master Address File (MAF). The MAF contains important information about all households in the United States. However, the MAF must add and delete addresses every five years based on the habitability of households. Consequently, this process is extremely costly for the Census Bureau. Statistical methodologies are being developed to help predict the changes in habitability using a large number of predictors. This will eliminate the need for the costly AdCan operation. Adragni et al. proposed a methodology called Minimum Average Deviance Estimation or MADE. It is based on the concept of local regression and embeds a sufficient dimension reduction of the predictors. The methodology was developed for response variables from the exponential family distributions and was implemented in R.

The goal of this project is to evaluate the performance of MADE on ultra high dimensional data through simulations. The first step is to parallelize several snippets of the MADE R-script in order to help the code run faster and to analyze the speed-up of these parallelized snippets compared to their serial alternatives. Simulated data with increasing large dimensions will be used to evaluate the runtime under specified hardware setups. In doing this, a limited stress test will be performed to determine how large of a data set UMBC's High-Performance Computer (HPC), maya, can handle. Finally, we will compare two prediction procedures that are devised under MADE. The results of these tests allow evaluating the capabilities of MADE which may help the US Census Bureau to predict the additions and deletions to MAF.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Graduate assistant Elias Al-Najjar was supported during Summer 2015 by UMBC.

### AN APPROACH TOWARDS EFFICIENT CANCER IMMUNOTHERAPY

## Sarah Pollock, Danielle Schmitt, Songon An, Minjoung Kyoung Department of Chemistry and Biochemistry, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Developing successful cures and treatments for cancer has continued to elude scientists for many decades. A promising and relatively new field of study called Cancer Immunotherapy employs the immune system to kill target cancer cells. Cancer Immunotherapy can be improved by a better understanding of the mechanisms of immune cells and how they alter the biology of target cancer cells, resulting in apoptosis.

The immune system is a crucial part of a host's biological response towards protecting the body from infection. Within the immune system, there are three types of white blood cells, with the focus of this project on a specific type, lymphocytes. Natural killer (NK) cells are a type of cytotoxic lymphocyte, which destroy target cells by the release of cytotoxic granules and interferons. This project is exploring the field of Cancer Immunotherapy by studying the mechanisms involved when NK cells kill cancer cells and determining which metabolic and signaling pathways of the cancer cells are altered. We are interested in looking at the glycolysis and gluconeogenesis as well as the purine biosynthetic pathway. Our target cells are HeLa cells and the breast cancer line, Hs 578T.

Current work has focused on identifying a library of commercially available compounds secreted by the NK cells to determine how these components affect the target cells. We will visualize the interaction between the secreted compounds and live cancer cells in real-time. Ultimately this project will shed light on how NK cells are interrupting the metabolic pathways of cancer cells.

This investigation was supported <in part> by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences and UMBC startups and UMBC-Special Research/Assistantship Initiative Support (SRAIS) award.

#### MAP1B IMPACTS ON NEURULATION AND MICROTUBULE STABILITY

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Brain development is a stepwise process that begins with neurulation. It is the process by which the neural tube develops, the precursor to the brain and spinal cord. Disrupting the intricate process of neurulation can result in mild to severe neural birth defects. An important and conserved event in neurulation is neural convergence extension (NCE) of the neural ectoderm. During NCE, neuroepithelial cells elongate mediolaterally and migrate towards the midline, thus narrowing and lengthening the neural plate. An important cellular component that drives NCE are microtubules (MTs). MTs are dynamic cytoskeletal tracts that drive tissue morphogenesis. Insufficient regulation of microtubule dynamics during neurulation is associated with neural tube defects in model organisms. MTs shorten, lengthen, and stabilize at the instruction of intrinsic and extrinsic factors to shape the tissues using cellular processes that are poorly understood. One such process is regulation by Microtubule Associated Proteins (MAPs), which bind directly to microtubules. Most MAPs control dynamics and stability. Specifically, Map1b temporally modulates MT polymerization and axon elongation, crucial aspects of early nervous system development.

In the direction of better understanding Map1b and its impacts, MO and Dominant Negative (DN) constructs were used to generate Map1b loss of function (LOF) phenotypes in zebrafish embryos. We found that depleting Map1b with MOs delayed NCE. Histological examination of the MO experiments showed that Map1b depletion caused destabilization in microtubule lattices and altered cell morphology during NCE. Our results are congruent with others that markedly implicate Map1b as a key microtubule regulator during neural tube morphogenesis.

After the alleged invalidation of MOs in recently published paper, we began using RNA Dominant Negatives (DN) to knock-out Map1b. Preliminary results from our dominant negative study are forthcoming, however, we anticipate agreement with the MO study.

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Notes:

\*These authors contributed equally to this work

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#### GENOMIC RECOGNITION OF HUMAN IMMUNODEFICIENCY VIRUS AND ITS RELATIVES

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The Human Immunodeficiency Virus (HIV) is still infecting millions of people worldwide, with significant prevalence in the U.S.; however, our knowledge about HIV replication, which includes genome recognition, is limited. This genome recognition step occurs when two strands of RNA dimerize and bind to the viral protein nucleocapsid (NC).

To characterize genome recognition in HIV, we selected the Simian Immunodeficiency Virus of chimpanzees  $(SIV_{cpz})$  as our comparative animal model.  $SIV_{cpz}$ , from which HIV was transmitted, is structurally and genetically similar to HIV, but it contains different sequences within the Dimer Initiation Site (DIS) stem loop, an important component of the viral RNA for genome recognition.

We prepared the isolated DIS stem-loops of  $SIV_{cpz}$  and HIV strains and characterized the dimerization behavior of these DIS stem-loops using native gel electrophoresis. Our time-dependent and concentration-dependent analyses show that increasing RNA concentration and incubation times promote dimerization in  $SIV_{cpz}$  and HIV. In addition, the interactions between NC and the RNA also promote dimerization in  $SIV_{cpz}$  and HIV. Overall results have indicated that  $SIV_{cpz}$  and HIV-2 DIS constructs are more labile than HIV-1 DIS. A better understanding of genome recognition provides useful information for anti-retroviral drug development.

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## IMPACT OF CALCIUM STORE OVERLOAD ON ELECTRICAL DYNAMICS OF CARDIAC MYOCYTES

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Heart disease is the leading causes of mortality in the United States. One cause of heart arrhythmia is calcium mishandling in cardiac muscle cells. We are presenting a mathematical model of the mechanism by which calcium waves propagate through cardiac muscle, or cardiomyocytes. This mechanism involves calcium being released from the sarcoplasmic reticulum (SR) through calcium release units (CRUs) in sparks. These sparks can cause other CRUs to release calcium, producing waves of calcium throughout the cell. The mathematical model is coded in C and run using parallel computing to efficiently generate simulations of the model; Matlab is utilized to create images indicating the calcium concentration throughout a cardiac cell with respect to time. Our model accounts for changes in the calcium concentration of the SR, the effects of buffers in the SR, particularly calsequestrin and other SR buffers, and the effects of voltage across the cell membrane. We have found that incorporating a dynamic SR calcium concentration causes the flux of calcium through open CRUs to taper off over the duration of the CRU firing, ultimately lowering the likelihood of waves to propagate. Likewise, including the effects of calcium buffers in the SR decreases the free calcium concentration, again affecting the likelihood of waves to propagate. Additionally, voltage-gated channels are utilized to examine the impact of calcium dynamics on voltage across the membrane.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing hpcreu.umbc.edu in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos.~CNS--0821258 and CNS--1228778) and the SCREMS program (grant no.~DMS--0821311), with additional substantial support from UMBC. Co-author Michael McCauley was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Zana Coulibaly was supported during Summer 2015 by UMBC.

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## COMPARISON OF PERFORMANCE ANALYSIS TOOLS FOR PARALLEL PROGRAMS APPLIED TO CombBLAS

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Performance analysis tools, or profilers for short, can be powerful tools for high performance computing. When a computer program is running slowly, it may be difficult to tell, where the bottleneck is located in the code, in particular if the code is a parallel program. By breaking it down to how long the CPUs are taking on each process (profiling) or showing when events take place on a timeline over the course of running a program, a performance analysis tool can tell the programmer exactly, where the computer is running slowly. With this information, the programmer can focus on these performance "hotspots," and the code can be optimized to run faster.

We compare the performance analysis tools TAU, ParaTools Threadspotter, Intel VTune, Scalasca, HPCToolkit, Score-P, when applied to the example of CombBLAS (combinatorial BLAS), a C++ algorithm in the GraphBLAS set of graph algorithms using BLAS (Basic Linear Algebra Subroutines). Using these results, we improve the implementation of CombBLAS and show performance data obtained on the distributed-memory cluster maya in the UMBC High Performance Computing Facility.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-authors Wesley Collins and Daniel Martinez were supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Ari Rapkin Blenkhorn, Jonathan Graf, and Samuel Khuvis were supported during Summer 2015 by UMBC.

## DEVELOPMENT OF A LOW-COST AEROSOL SENSOR FOR DISTRIBUTION IN HIGH DENSITY NETWORKS

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Concern for air quality has garnered attention in recent years due to studies revealing the adverse effects of poor air quality on health. Thus, monitoring air quality on the personal scale has become more important to assess individual pollutant exposure. To address this problem, there has been a recent effort to create low-cost monitors that can be deployed in a high density network to map air pollution in urban areas, where high spatial gradients are known to occur. The objective of this work is to develop a low-cost aerosol sensor. The major sensor components are a Shinyei (PPD42NJ) dust sensor and an Arduino Uno for control and data logging. The approximate cost of our current prototype is \$40, significantly less than typical monitors that cost thousands of dollars. The system is also extremely small, currently housed in a 7.5x4.25x2.25 inch enclosure, which offers potential for portability. Prior to deploying this system to monitor air quality, the sensor needs to undergo rigorous validation. We have begun this process by placing the sensor through a series of tests designed to characterize the instrumentation as well as discern the dust sensor's usability and limitations. Zero-air, which lacks particulate matter, was run through the machine as a test for no signal. Rosin smoke was used to induce a signal by creating an overabundance of particles in the air. So far, the results of these experiments look promising, and the dust sensor reacts in predicted ways. Future work will focus on ensuring the accuracy of our device by utilizing professional equipment to calibrate our sensor for field measurements. Once we have a firm understanding of the measurement capabilities of the device, we will then focus on deploying the sensor to characterize air in locations of interest then work to improve air quality in that area.

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## APPLYING THE DIMER EFFECT MIXING MODEL FOR SPATIAL SPECIFICATION OF GENE EXPRESSION

## <u>Tiana Boardley</u><sup>1</sup>, Fernando Levstein<sup>2</sup>, and Mauricio Bustos<sup>1</sup> <sup>1</sup>Department of Biology, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>2</sup>FAMAF-UNC, Cordoba, Argentina.

In order for the development of complex shapes and functions to occur in multicellular organisms, spatial and temporal cues must drive selective expression of genomic information. A dimer effect mixing model created by Bustos and Levstein describes how segmentation gene expression in early Drosophila embryos is specified by eight key transcription factors. The model calculates a regulation function (freg) of the transcription factors' abundances that matches the *in* vivo expression pattern of mRNA expression driven by a cis regulatory module. A canonical model, is a hypothetical model comprising every possible dimer that could be formed with the eight base transcription factors. Here, we show that by including different subsets of transcription factor dimers a potentially large number of non-canonical models can be built for any gene expression pattern. We also demonstrate a special class of "simplified," non-canonical models and some of their common features. To construct simple models that are realistic, a new project will be initiated to data mine the published literature in search of all experimental evidence supporting the existence of transcription factor dimers. Moreover, simplified, noncanonical models will provide a starting point to learn how the DNA sequence of a module serves as a template that guides the correct cohort of transcription factor dimers to capture RNA polymerase and initiate gene expression.

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#### TIME-RESOLVED PUMP-PROBE REFLECTIVITY

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A pump-probe experiment is often used to study ultrafast carrier dynamics in semiconductors. To carry out these high-speed measurements it is important to know the duration of the excitation laser pulse. Autocorrelation measurements are used to estimate the laser pulse duration and involve a series of steps. First, the beam is split into two separate paths. Mirrors are then arranged so that the beams are parallel and within a few millimeters of each other and the path lengths identical. Then, the beams are focused onto a beta barium borate nonlinear crystal. A stepper motor is used to adjust the position of a mirror, which results in the appearance of a third beam, the desired autocorrelation signal between the two beams. The third beam is directed towards a photodetector which is connected to a lock-in amplifier and a computer program (LabVIEW). The program records the data and plots a graph of the amplitude of the pulse versus the time delay. The pulse duration was estimated to be 6.27 picoseconds, in excellent agreement with the manufacturer of the Nd:Vanadate laser.

In a time-resolved pump-probe reflectivity experiment of a semiconductor (InGaAs), an ultrashort laser pulse is split into two portions; a stronger beam (pump) is used to excite photocarriers in the semiconductor and a weaker beam (probe) is used to monitor the time dependent change of the reflectivity of the sample. Measuring the changes in the reflectivity as a function of time delay between the arrival of pump and probe pulses yields information about the photocarrier lifetime of the sample. Time-resolved pump-probe experiments permit the measurement of the photocarrier lifetimes of different materials to be evaluated and helps one decide which material is best for different optoelectronic applications.

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## PARALLELIZATION FOR FAST IMAGE RECONSTRUCTION USING THE STOCHASTIC ORIGIN ENSEMBLE METHOD FOR PROTON BEAM THERAPY

REU Site: Interdisciplinary Program in High Performance Computing <u>Fernando Avila-Soto<sup>1</sup>, Alec Beri<sup>2</sup>, Eric Valenzuela<sup>3</sup>, Abenezer Wudenhe<sup>4</sup>,</u> Graduate assistants: Ari Rapkin Blenkhorn<sup>4</sup>, Jonathan S. Graf<sup>5</sup>, Samuel Khuvis<sup>5</sup>, Faculty mentor: Matthias K. Gobbert<sup>5</sup>, Client: Jerimy Polf<sup>6</sup> <sup>1</sup>Department of Computer Science and Mathematics, Muskingum University <sup>2</sup>Department of Computer Science, University of Maryland, College Park <sup>3</sup>Department of Computer Science, California State University, Channel Islands <sup>4</sup>Department of Computer Science and Electrical Engineering, UMBC <sup>5</sup>Department of Mathematics and Statistics, UMBC <sup>6</sup>Department of Radiation Oncology, University of Maryland School of Medicine

Proton beam therapy is becoming increasingly common in the field of cancer treatment because of the advantages over other forms of radiation therapy. This advantage arises from the finite range of the proton beams and the relatively low dosage of radiation upon entering a patient and large spike in dose at the end of the beam range known as the "Bragg peak". By carefully controlling the beam range, the high dose Bragg peak can be used to target tumors while minimizing irradiation of surrounding healthy tissue. Research is currently underway to develop methods to image the proton beam as it passes through the patient as a means of verifying that the Bragg peak is irradiating the tumor as intended. As part of this research, a new computer code has been developed that use the stochastic origin ensemble method to reconstruct an image of the gamma radiation produced by the proton beam. From this image, the behavior of the proton beam in the patient can be studied and verified, i.e., it can be used to predict if the treatment beam is delivering dose correctly at each depth in the patient.

The objective of this research study is to significantly decrease the run time of the given computer code. For the reconstruction algorithm to be useful in medicine, it must be fast and precise, since it is impractical to ask that a patient lie completely still for several minutes. Thus, parallel computing techniques are being applied to the source code for optimizing experimental image reconstruction speed on the UMBC High Performance Computing Facility.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Gabrielle Salib was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Ari Rapkin Blenkhorn, Jonathan Graf, and Samuel Khuvis were supported during Summer 2015 by UMBC.

## THE PERFORMANCE OF IRRITANT-EXPOSED WILDTYPE AND SKN-1A KNOCKOUT MICE IN A COOKIE TEST WITH ODOR BACKGROUND

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## CHARACTERIZING MATRIX'S ROLE IN PACKAGING tRNA<sup>Lys3</sup> IN HIV-1 VIRIONS THROUGH SITE-DIRECTED MUTAGENESIS OF BASIC PATCH RESIDUES

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Upon infection of a CD-4 cell, the RNA genome of HIV is reverse transcribed into DNA. The initiation of this process requires a host cell tRNA<sup>Lys3</sup> to act as a primer and bind to the primer binding site of the genomic RNA, allowing for elongation of the complementary strand. After non-specific integration and subsequent transcription of the intermediate, the unspliced variant of the resultant RNA can be translated into gag and gag-pol proteins. The N-terminal of this polyprotein is functionally characterized as the matrix domain which is quintessential for plasma membrane targeting and binding as well as the assembly and budding of immature virion. Further, past studies have shown that the matrix domain binds to RNAs, the majority of which are tRNAs, via the same highly basic region. The previously mentioned tRNA<sup>Lys3</sup>, though found at a relatively low concentration in the cell, binds with a high frequency. This suggests that matrix may play an integral role in packaging tRNA for further use during reverse transcription.

Based on these previous reports, our goal is to structurally characterize matrix and tRNA interactions through the use of Electrophoretic Mobility Shift Assays (EMSA). Specific tRNA-matrix binding has been further supported by EMSA. In order to determine which residues are important for binding, we have constructed mutants of the matrix protein at residues which have been previously reported to be integral for specific non-promiscuous binding to PI(4,5)P<sub>2</sub> containing membranes. The mutant construct K29A did not show a significant decrease in tRNA binding while the K29, 31A construct needs to be studied further. Direct structural implications of the binding will be studied via HSQC in the future.

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## REMOTE SENSING MONITORING OF CANADIAN WILDFIRE SMOKE AND ITS IMPACT ON BALTIMORE AIR QUALITY

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High spatial and temporal resolution Elastic *light detection and ranging* (lidar) measurements allows to monitor long-range transport of particulates, such as dust and smoke, that impact local and regional air quality. These lidar measurements enhance current knowledge and understanding on how vertical layering and long range transport of natural and anthropogenic particle pollution may alter the relationship between column aerosol optical depth and surface particle pollution concentrations. The impact of a strong haze event in June 9-11, 2015 is examined. Particle pollution associated to this event yielded a 245% increase in aerosol optical depth values compared to the average mean June values for the last decade. We present how air mass back trajectory analysis, aerosol intensive and extensive parameters from lidar, sun-photometer and satellite observations revealed the presence of Canadian wildfire smoke impacting the Baltimore air quality.

The research is supported by NOAA-CREST/CCNY Foundation CREST Grant-NA11SEC481004.3 and the Joint Center for Earth Systems Technology.

#### PH-DEPENDENT ABSORBANCE BEHAVIOR OF ANTIBIOTIC PHARMACEUTICALS

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The use of antibiotic pharmaceuticals in human and agricultural applications has led to the increased detection of these antibiotics and their metabolites at trace concentrations in drinking water and wastewater around the world. The ubiquitous presence of antibiotics has led to negative impacts on the environment, including development and spread of antibiotic resistant bacteria in the environment. UV-irradiation has been shown to degrade antibiotics. While UVbased treatment methods are promising due their current use in disinfection and the high photoreactivity of certain classes of antibiotics, knowledge of the pH-dependent absorbance behavior is still needed to characterize photodegradation kinetics. The purpose of this project was to model pH-dependent molar absorptivity (or molar extinction coefficients) of at least 15 commonly prescribed antibiotic pharmaceuticals in the wavelength range of 220-900 nm. The absorbance of antibiotics was measured at pH 2–12 using 10 mM phosphate buffer. Preliminary results for organoarsenical antibiotics showed pH-dependent variation of molar absorptivity due to acid/base speciation. Acid dissociation constants for antibiotics were obtained from literature. The specific molar absorptivity for each individual species was determined by fitting observed data to a speciation-based model. The data were condensed into a concise and effective database for laboratory use. This database will be employed to study the photolytic fate of these antibiotics in engineered systems and natural environments. Ultimately, the project will contribute to the design of engineered systems for effective treatment of antibiotic-contaminated water and wastewater streams.

This project was possible through the efforts of the Park School Internship Program, UMBC, and the Department of Chemical, Biochemical, and Environmental Engineering.

## COPPER BIOREMEDIATION USING GENETICALLY ENGINEERED ESCHERICHIA COLI

<u>Alex Kuznetsov<sup>1</sup></u>, <u>Natithorn Bhusri<sup>1</sup></u>, UMBC iGEM team<sup>2</sup>, Cynthia Wagner<sup>3</sup>, Stephen Freeland<sup>4</sup> <sup>1</sup>Department of Chemistry and Biochemistry, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>3</sup>Department of Biology, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250 <sup>4</sup>Department of Interdisciplinary Studies, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

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Copper is a major pollutant in a variety of freshwater ecosystems. When copper is oxidized from  $Cu^+$  to  $Cu^{2+}$ , it often produces a free radical known as a reactive oxygen species (ROS), which is capable of severely damaging biological molecules. *E. coli* have the ability to uptake copper, but after a certain threshold, the copper becomes toxic to the cell. Due to the toxicity of copper, *E. coli* quickly saturate and are unable to uptake more than a small amount of copper.

Our goal is to increase the efficiency of copper uptake in *E. coli* for the purpose of bioremediation in freshwater ecosystems. We engineered *E. coli* to express the yeast CUP1 gene in an attempt to increase copper tolerance. CUP1 encodes a metallothionein protein that binds 11 copper atoms, thereby preventing formation of the ROS. In addition, metallothionein detoxifies hydroxyl radicals with its cysteine groups.

Through the use of growth curves and an assay to measure copper uptake, we will present our preliminary data on *E.coli* transformed with the CUP1 gene as our initial attempt to create a bacterial strain that has a higher resistance to copper toxicity.

The UMBC iGEM Team would like to acknowledge the UMBC Student Government Association, the UMBC College of Natural and Mathematical Sciences, UMBC Biology Department and UMBC Chemistry and Biochemistry Department for their financial support without which our project would not be feasible. We would also like to acknowledge Dr. Stephen Mang for his support with copper measurement.

#### EVOLUTION AND STRUCTURE OF NIGHT TIME WAVES AND BORES

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The Plains Elevated Convection at Night (PECAN) field campaign is a multiagency project (DOE, NSF, NASA, NOAA) in collaboration with national and international universities. The campaign is designed to understand the conditions that lead to convection initiation of thunderstorms and the evolution and lifecycle of largescale systems at night. Understanding the initiation and evolution of convective systems will lead to an explanation of the observed night time maxima in summer precipitation over the central plains and help improve nation's forecasting and weather prediction capabilities. PECAN has four themes of research, which includes: documenting night time bore wave disturbances, Nocturnal mesoscale convective systems (MCSs), Nocturnal convective initiation (CI), and evolution and character of the low level Jet (LLJ). The University of Maryland Baltimore County deployed their research instrumentation at the FP2 site in Greensburg, KS. Data was collected from different instrumentation that consisted three types of lidars: Raman lidar, Doppler wind lidar, and the Elastic lidar. Other instruments operated at the site include the MicroWave Radiometer (MWR), Radiosondes, and an x-band radar (named X-BADGER) was also operated in order to document the variabilities in the nighttime atmosphere. This study will use data from PECAN (June 1 to July 15, 2015) and investigate the occurrences, evolution and structure of undulare Bore and build a statistics at FP2, in Greensburg, KS.

The research is supported by NOAA-CREST/CCNY Foundation CREST Grant-NA11SEC481004.3 and the Joint Center for Earth Systems Technology.

## CHARACTERIZATION OF PHTHALATES BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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Phthalates are a family of chemicals used to make vinyl and plastics softer and more flexible. Though useful, many species or variations of phthalates pose health risks such as being carcinogenic and long term exposure to diisononyl phthalate can cause reproductive issues and birth defects. It is important to inform consumers when potentially harmful phthalates are present in products. Phthalate-free products already exist; however, making everything phthalate-free would be highly costly and time consuming. Researchers strive to find more accurate ways to characterize phthalates to determine the health risks they might carry. Gas Chromatography–Mass Spectrometry (GC-MS) is an analytical instrument that is well-suited for the separation and detection of phthalates.

GC-MS is used to identify different volatile substances within a sample by separating substances into the gas phase. The sample is then sent through a column and is separated based on physical properties of the molecule. Once separated, the analytes enter into the MS, which ionizes and breaks apart the analyte, producing a mass spectral fingerprint of the compound of interest. The information from the GC-MS can be used to characterize phthalates based on their structures.

Before starting the project branched and unbranched phthalates were synthesized to act as model compounds. The non-branched samples are expected to have a longer retention time because they have a higher surface area (boiling point) than the branched phthalates. Then the samples of controlled mixtures of branched and unbranched phthalates were then produced and analyzed with GC-MS. The intent is to find a correlation between the two phthalate controls and unknown branching phthalates. The information gathered from the GC-MS will help in characterization of this class of compounds. This has potential to be a step forward into identifying and better understanding the health risks of phthalates.

I would like to thank Suze Nathalie, my chemistry teacher at Mergenthaler for telling me about this program and signing me up for it. Also, I want to thank YouthWorks for paying me and providing transportation to and from UMBC. Thank you to Justine Johnson for running the summer program. Finally, a huge thank you to Dr.LaCourse and the MCAC staff for allowing me to work on project under them.

#### THE BINDING OF FIV MA TO MIMETIC MEMBRANES

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The feline immunodeficiency virus (FIV) is a lentivirus that weakens the immune system of the infected cat, similar to the effects of the human immunodeficiency virus in humans. The assembly process is vital to the retroviral replication cycle because the Gag polyprotein (Gag) is targeted to the plasma membrane of the host cell during this stage. The component of Gag that mediates its transportation and interaction with the plasma membrane is the matrix domain (MA). The proposed extended lipid binding model demonstrates how HIV-1 MA binds to the plasma membrane. The limitations in this proposed model are the purpose behind our studies: truncated lipids were used in this study, but we strive to use the native lipid to better characterize binding. This work investigates how FIV MA operates in targeting and binding to the lipid phosphatidylinositol-(4,5)-bisphosphate [PI $(4,5)P_2$ ] with the use of liposomes as mimetic membranes. Our reasoning behind studying the virus in cats is that, like HIV Gag, FIV Gag binds to PI(4,5)P<sub>2</sub>, many cats are already infected with the virus so the risk of unnecessary harm for research purposes is reduced, and unlike simians, it is inexpensive to house and maintain cats during study. Nuclear magnetic resonance spectroscopy (NMR) is used to qualitatively analyze the binding interaction between FIV MA and PI(4,5)P<sub>2</sub>. Comparison of membrane targeting in FIV MA and HIV-1 MA may support application of household cats as animal models for the treatment of HIV. In addition to studying the assembly process, great focus is placed on efficiently preparing protein for NMR studies by developing a new concentrating protocol.

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## UNDERSTANDING THE ROLE OF PASSENGER GENES IN THE BMT PROSTATE CANCER MODEL

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#### PERFORMANCE STUDIES OF THE BLOSSOM V ALGORITHM

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The Blossom V algorithm is an important algorithm used in graph theory to compute a perfect matching of minimum cost of a graph. Graph theory allows for effective modeling of real-world scenarios. With growing amounts of data, the fast speed of algorithms becomes imperative to their efficiency. Performance studies were run on the maya cluster in the UMBC High Performance Computing Facility to investigate the performance of the algorithm on graphs of various sizes and orders. Various time measurements and total memory usage were recorded for the different graphs. Several memory profilers, such as Valgrind, were used to determine memory usage. Systematic studies for a variety of sizes and orders are used to analyze the total execution time and memory usage of the algorithm. The execution time increases steadily with the size and order of the graphs, and we can pinpoint the location of major portions of execution time. Also memory usage increases steadily with the size and order of the graphs, as memory usage is largely attributed to the size of the structures used to store the vertices and edges of the graph. The results of the performance studies indicate areas of the algorithm that will benefit from potential parallelization. Future research may include development of a parallel implementation of the Blossom V algorithm in order to improve execution time. Furthermore, potential techniques to reduce memory consumption should be explored.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Gabrielle Salib was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Ari Rapkin Blenkhorn, Jonathan Graf, and Samuel Khuvis were supported during Summer 2015 by UMBC.

#### ROLE OF SECRETORY PATHWAY PROTEINS ON CELL MIGRATION

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Migratory cells have a central role in embryonic development, the immune response, and cancer metastasis. However, the molecular mechanisms behind the events signaling and mobilizing a cell for migration are not fully understood. We use Drosophila melanogaster, which provides an important model system for identifying and manipulating genes involved in migration. Border cells in the Drosophila ovary acquire migratory properties, providing a tractable model for investigating the genetic and cellular mechanisms behind migration. Anterior polar cells of the developing egg chamber secrete the ligand Unpaired, which activates the Janus Kinase/Signal Transducer and Activator of Transcription (JAK/STAT) pathway. Activated JAK activates STAT, which functions as a transcription factor. In Drosophila border cells, this specifies them for migration. Proteins of the secretory pathway have been previously shown to be important in Unpaired secretion from the polar cells. Here we investigate the role of protein transport in vesicles for exocytosis and between organelles in both polar and border cells. In polar cell specific knockdowns of secretory pathway proteins, we expect to see a severe defect with little to no border cells specified due to a loss of secretion of the ligand Unpaired, while the effects of border cell specific knockdowns are unknown. Reporter gene analysis for Sar1 and Sec23, proteins involved in vesicle trafficking, revealed no distinct expression pattern for either line. In other experiments, we selectively knocked down the secretory pathway genes Sar1, Sec23, Sec16, Membrin, and Garz via RNA interference and overexpressed Sec23 in motile cells to look for any defects in cell migration. Analysis of mutations in the secretory pathway can provide new insights into the genes involved in specifying and maintaining the fate of migratory cells, and has broad implications for understanding migratory pathways in immune response, metastasis of cancer, and other developmental disease.

This work was funded in part by the National Science Foundation Career Award to Michelle Starz-Gaiano, Ph.D.

# STATISTICAL ANALYSIS OF A CASE-CONTROL ALZHEIMER'S DISEASE: A RETROPECTIVE APPROACH WITH SUFFICIENT DIMENSION REDUCTION

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Alzheimer's Disease is a neurological disorder chiefly present in the elderly that affects functions of the brain such as memory and logic, eventually resulting in death. There is no known cure to Alzheimer's and evidence points to the possibility of a genetic link. This study analyzes microarray data from patients with Alzheimer's disease and disease-free patients in order to evaluate and determine differential gene expression patterns between the two groups. The statistical problem stemming from this data involves many predictor variables with a small sample size, preventing the use of classical statistical approaches from being effective. We turn to a novel three-step approach: first, we screen the genes in order to keep only the genes marginally related to the outcome (presence of Alzheimer's); second, we implemented a sparse sufficient dimension reduction to retain only predictors relevant to the outcome; lastly, we perform a hierarchical clustering method to group genes that exhibit mutual dependence. We adapted this methodology from Adragni et. al and expand on their work by optimizing the existing R code with parallel capabilities in order to enhance performance speed. Thus, our results reflect both an analysis of the microarray data and a performance study of the modified code.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Meshach Hopkins was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Elias Al-Najjar was supported during Summer 2015 by UMBC.

#### EXAMINATION OF THE ROLE OF THE GENE SHEP IN CELL MIGRATION

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Cell migration is an important area of scientific investigation as it is required for proper embryonic development, healing of injuries, and fighting against infection in organisms. While cell migration has these positive roles, it is also the mechanism responsible for cancer metastasis. In an attempt to obtain a full understanding of this process, we use the model organism Drosophila melanogaster because the genes regulating cell migration in flies are largely conserved in humans. The ovaries in the female fruit fly contain egg chambers that require a set of cells, called the border cells, to migrate for proper egg development. Previous work has shown that a gene called *shep* is expressed in the border cells. This gene encodes an RNA-binding protein that regulates gene expression post-transcriptionally. Preliminary studies suggest that loss of shep delays border cell migration. To test these findings, we used a D. melanogaster mutant that has an insertion of a reporter in the gene to observe where *shep* is expressed in the egg chambers. We also used mutants that have insertions which result in knockdown of the gene's function. This will allow us to observe any effects on border cell migration. We expect to find that *shep* does have a role. It is possible that the RNA-binding protein encoded by *shep* regulates miRNA function and therefore, participates in a known regulatory process such as the JAK/STAT pathway. Future research may reveal the exact means by which *shep* regulates cell migration in Drosophila, leading researchers to explore possible implications for similar RNAbinding proteins in human cell migration.

This project was funded in part by a National Science Foundation Career Award to Michelle Starz-Gaiano, Ph.D.

# CHARACTERIZATION OF FIV MYRISTYLATED MATRIX BINDING TO MIMETIC MEMBRANES

## <u>Colin O'Hern, Paige Canova</u>, Janae Baptiste, Dr. Michael F. Summers Howard Hughes Medical Institute, Department of Chemistry and Biochemistry, UMBC, 1000 Hilltop Circle, Baltimore, Maryland 21250

Feline immunodeficiency virus (FIV) is a retrovirus, similar to human immunodeficiency virus type 1 (HIV-1) in humans, that suppresses and inhibits activity of the immune system in cats. Approximately 2.5-4.4% of household cats are infected with FIV worldwide with symptoms including poor coat condition, gingivitis, diarrhea, and progressive weight loss. Studying FIV assembly is significant because humans and cats have similar immune responses, presenting a plausible target in an animal model for development of HIV-1 treatment. The Gag polyprotein consists of the following major domains: matrix (MA), capsid, and nucleocapsid. The proposed extended lipid binding model of HIV-1 depicts the interaction between MA and phosphatidylinositol-(4,5)-bisphosphate [PI $(4,5)P_2$ ], a phospholipid found in the plasma membrane; however, a limitation of this study was the use of truncated  $PI(4,5)P_2$ . The objective of this work is to use the native lipid to study its interaction with FIV MA. Liposomes, artificial lipid bilayers, are constructed that have compositions similar to that of the plasma membrane. Liposome binding assays employ nuclear magnetic resonance spectroscopy (NMR) to characterize the binding of FIV MA to PI(4,5)P<sub>2</sub> and draw comparison to interaction between HIV-1 MA and PI(4,5)P<sub>2</sub>. In addition, FIV MA has a large unstructured portion on the Cterminus that may aid in instability, so, by using mutagenesis to remove that region, it is proposed that the FIV MA stability will be increased, resulting in improved NMR data.

Howard Hughes Medical Institute, NIH/NIAID 5R37AI030917

## ROLE OF MATRIX'S LYSINE 31 IN PROMOTING tRNA<sup>Lys3</sup> PACKAGING IN HIV-1

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Upon entry in a host cell, the HIV-1 RNA genome is reverse transcribed into double stranded DNA by reverse transcriptase using human tRNA<sup>Lys3</sup> as a primer. Packaging of virions starts with the recognition of an unspliced viral RNA by Gag and GagPol proteins, which form a complex that is targeted to the plasma membrane (PM) by the matrix (MA) domain on the Gag protein. In addition to viral machinery, cellular tRNA<sup>Lys</sup> isoacceptors are also packaged. Interestingly, the tRNA<sup>Lys3</sup> primers abundantly bind to MA in cells, this binding however, greatly decreases within the virion. It has been hypothesized that RNA binds to the Highly Basic Region (HBR) of MA, inhibiting its myristoyl group and thus enhancing MA's ability to discriminate between membranes. Since tRNA<sup>Lys3</sup> is selectively packaged, we hypothesize that tRNA<sup>Lys3</sup> binds MA during packaging and regulates MA binding to  $PI(4,5)P_2$  in the PM. We plan to characterize the structure of the MA-tRNA complex using NMR and determine the residues involved in this interaction using mutagenesis studies. Due to previous studies done on the myristate and HBR we chose to investigate further the role of Lysine 31. We used a site-directed mutagenesis approach to create the K31A mutant. We successfully purified MA HBR mutant K31A through ion exchange and size-exclusion chromatography. The binding properties of the mutant protein to tRNA<sup>Lys3</sup> will be subsequently studied through gel shift assays and isothermal titration calorimetry.

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#### ANALYSIS OF FILTERS BY FOURIER TRANSFORM INFRARED (FT-IR)

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The average adult is made of up to 60% water.<sup>1</sup> It is important to make sure that the water humans are drinking is clean. Studies have shown over 1.8 million people die every year from contaminated water.<sup>2</sup> The Fourier Transform InfraRed(FT-IR) Spectrometer can help identify what is in the water humans drink. FT-IR measures molecular structure and the stretches allow for identification of functional groups which can help identify molecular structure. Stretches in a molecule show the specific frequencies that correspond with specific energy levels. FT-IR is used in many different sciences such as chemistry, biology and environmental science for various applications.

The goal of this project is to develop a simple approach of monitoring water contaminants using FT-IR. Preliminary experiments consist of testing different types of filters made up of various material (e.g. PVDF, PTFE, Nylon). The filter with the cleanest background will then be chosen for further experiments. 18M $\Omega$  purity water will be spotted, then dried with nitrogen gas (N<sub>2</sub>). And the filter will then be analyzed with the FT-IR. It is expected that the spotted filter will not look significantly different from the clean filter, because the water is certified pure. Then the 18M $\Omega$  water will be spiked with phthalates. A phthalate is a contaminant that is found in water from plastic. They are carcinogenic and can cause reproductive issues to women.<sup>3</sup> The spiked water will be filtered and analyzed. The unused filter serves as a control. Preliminary results show analysis of the filter is a viable way to analyze various impurities. By using this method one should be able to tell if a water system is contaminated with some insight into the contaminants identity.

I would like to give a big thank you to my teacher for giving me this opportunity to be a part of the MCAC research program. I would also like to thank the entire MCAC staff for helping with whatever I needed help with and allowing me to use their tools and instruments so that I could learn.

<sup>1</sup>http://water.usgs.gov/edu/propertyyou.html

<sup>2</sup>https://www.koshland-science-museum.org/water/html/en/Overview/Why-is-Safe-Water-Essential 3http://www.ehhi.org/reports/plastics/phthalates\_intro.shtml

#### **REV: THE REGULATOR OF VIRION EXPRESSION**

## <u>Geraldine Ezeka, Roald Teuben</u>, Jan Marchant, and Michael F. Summers Department of Chemistry & Biochemistry, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Human immunodeficiency virus, HIV, is a retrovirus that invades human CD4+ T cells by integrating its viral genome into the host cell's genome. Following this integration, an infected cell expresses viral accessory proteins from fully-spliced mRNA, which are exported from the nucleus via regular pathways. One such protein, Rev, facilitates a critical step in the viral replication cycle: the export of unspliced and singly-spliced viral mRNA from the nucleus to the cytoplasm. Unspliced mRNA acts as the genomic material of new virions, and also encodes for polyproteins necessary for their formation. In order to transport the mRNAs, Rev forms an oligomer on the Rev Response Element (RRE), a structural landmark located only on unspliced and singly-spliced mRNAs. The Rev-RRE complex initiates recruitment of the host's Crm1 nuclear export machinery. In order to better understand the molecular details of retroviral mRNA export, we plan to characterize the Rev-RRE interaction using a range of biophysical techniques including nuclear magnetic resonance (NMR) spectroscopy.

In order to express Rev, we used standard cloning techniques to insert the Rev gene into the pET-19b plasmid. We also introduced mutations to Rev to prevent oligomerization to aid in purification and NMR experiments. Previous studies have successfully characterized a similar construct of Rev in complex with a small portion of the RRE. However, there are few highresolution structural studies on Rev and the full RRE, primarily due to inherent difficulties in studying large RNAs. Our research aims to enhance the understanding of the interaction by forming a Rev-RRE complex with full length RRE and analyzing the interactions using NMR. Our findings will be used to elucidate the structural basis of Rev-RRE interactions to potentially guide development of therapeutics targeting this stage of the HIV-1 life cycle.

This work is supported by NIH/NIGMS grant #P50GM103297 and the Howard Hughes Medical Institute. We would like to thank Michael Summers for making our work possible and Jan Marchant for his guidance.

# ARCHITECTURAL DETAILS THAT MAKE NAVIGATION DIFFICULT FOR VISUALLY IMPAIRED INDIVIDUALS

### <u>Chuk Amaefule</u> and Amy Hurst Information Systems Department, UMBC,1000 Hilltop Circle, Baltimore, MD 21250

When a blind person is making their way around various locations, information about their surroundings is constantly being gathered to help them navigate. They use architectural details and cues such as changes in pavement textures, audible signs, and smells from a nearby restaurant to help determine their current location. We conducted focus groups and observations to observe how individuals with vision impairments navigate. We used the results to get a better understanding of how blind people navigate so we can design a navigation device that can help a them navigate around these obstacles safely without any major interference. Many of these various features and details that architects have implemented in the environment are meant to help however, there are many architectural details that make navigation difficult for a blind individual such as curb cuts, open spaces with no tactile or audible feedback, and sidewalks that are flush with the street. Some features are meant for accessibility but can make navigation unnecessarily difficult such as sidewalks that are flush with the street. They are in place to make it easier for riders to cross the street however, for people with vision impairments they may not detect it and can end up walking into oncoming traffic. Features like this can lead to an unsafe and problematic travel. Based on our studies, we find that a blind person obtains so much information from their surroundings that inconsistencies with tactile and audible feedback make it difficult to determine orientation, which leads to more interactions from sighted individuals and infringes on their ability to navigate independently. For certain areas such as intersections, we could campaign for all of them to be equipped with audible signs and ridges in the sidewalk, if it is flush with the street, to help visually impaired people navigate independently.

This research is supported by Toyota Motor Engineering & Manufacturing North America. Mentored by Michele Williams and Amy Hurst.

#### CHARACTERIZATION OF THE MONOMERIC HIV-1 RNA 5' LEADER

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Human Immunodeficiency Virus (HIV), a retrovirus which contains two copies of its RNA genome, is the causative agent of Acquired Immunodeficiency Syndrome (AIDS). HIV is a retrovirus which utilizes reverse transcriptase to reverse transcribe its RNA genome into DNA. Reverse transcriptase does not contain proofreading mechanisms, resulting in a high mutation rate. Currently, various drug therapies exist that target specific steps in HIV viral life cycle; however, finding new drug targets is vital due to the high mutation rate of the virus and noncompliance to strict drug regimens. The 5' leader (5'-L) is an untranslated region of the HIV-1 RNA genome, located at the 5' end, that controls translation and packaging through its structural conformation. The highly conserved nature of this region, unlike the rest of the genome, makes it a promising drug target. The 5'-L exists either as a monomer or dimer. The monomer is proposed to promote translation, while the dimer is selectively packaged into new viral particles.

This study utilizes nuclear magnetic resonance (NMR) techniques to characterize the monomeric structure of the 5'-L. NMR studies have allowed for confirmation of various predicted secondary structures within the monomeric 5'-L.

Because mRNA is capped *in vivo*, this study also investigates the effects of capping of the 5'-L. Native gel electrophoresis comparing the monomer-dimer equilibrium between capped and uncapped RNA show that the presence of the 5' cap stabilizes the monomeric conformation. Previous literature showed inconsistencies in the start site of the 5'-L. The current study examines the 5'-L to determine if the start site consists of one G, two Gs or three Gs.

Future studies will allow complete characterization of the secondary and tertiary structures of the 5'-L along with a further understanding of the implications of heterogeneity within the cell, regarding capping and start sites.

Emily Diaz was supported, in part, by a contract through the NIH/NIDA, UMBC, and the Meyerhoff Scholars Program.

## EFFECT OF RNA POLYMERASE I AND ACAT INHIBITION ON THE GROWTH OF ENZALUTAMIDE-RESISTANT PROSTATE CANCER

## <u>Megha Kori</u><sup>1</sup>, Michael Rubenstein<sup>1</sup>, Paul Sirajuddin<sup>2</sup>, Marikki Laiho<sup>2</sup>, Charles Bieberich<sup>1</sup> <sup>1</sup>Department of Biology, UMBC, 1000 Hilltop Circle, Baltimore, Maryland 21250 <sup>2</sup>Department of Radiation Oncology, Johns Hopkins University School of Medicine, 1550 Orleans Street, Baltimore, Maryland 21231

Prostate cancer is the second leading cause of death in American adult men: one in seven men will be diagnosed with this disease. Previous research has demonstrated that monotherapy is rarely a curative measure. Instead, a combinatorial approach results in significantly better clinical outcomes. BMH-21 is an RNA Pol I inhibitor and DNA intercalator that has been shown to activate antitumorigenic activity, while the ACAT inhibitor Avasimibe has demonstrated an ability to inhibit the growth of glioma cells by inducing apoptosis and decreasing the accumulation of cholesterol esters. Here, we describe a combination drug trial testing the effects of BMH-21 and Avasimibe on the growth of xenograft tumors in immunocompromised mice. Mice were injected daily with a combination of BMH-21 and Avasimibe, BMH-21 alone, Avasimibe alone, or a placebo. We monitored the rate of tumor growth and euthanized mice that presented with either severe weight loss or excessive tumor volume. Our results showed that the cohort injected with a combination of Avasimibe and BMH-21 had the lowest rate of tumor growth, however, this was not significantly less than the rate of tumor growth in mice treated with BMH-21 alone. Additionally, treatment with Avasimibe alone appeared to have caused an accelerated rate of tumor growth. A larger trial is currently in progress, as these results suggest a potential for the use of this combinatorial approach in the treatment of human prostate cancer.

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### NON-IMAGE FORMING VISUAL PIGMENTS: DO THEY INTERNALIZE?

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G protein-coupled receptors (GPCRs), the largest family of eukaryote transmembrane receptors, respond to extracellular stimuli and trigger a response within the cell. Opsins are specialized GPCRs that are involved in the conversion of light into a biological signal. Melanopsin is an opsin that is found in intrinsically photosensitive retinal ganglion cells (ipRGCs) in the mammalian retina and regulates non-image forming functions such as circadian photoentrainment and pupillary constriction. While much of the phototransduction pathway of melanopsin remains unknown, we hypothesize that melanopsin is internalized after activation by light and deactivation by  $\beta$ -arrestin. To test this hypothesis, we synthesized GFP-tagged melanopsin constructs in a mammalian expression vector, PMT3, through cassette mutagenesis and expressed these constructs in Human Embryonic Kidney (HEK293) cells. We then compared localization of melanopsin is internalized in a heterologous expression system.

This work was funded by NSF DBI-1031420.

# THE BENEFITS OF ARCHITECTURAL DETAIL INFORMATION IN NAVIGATION OF VISUALLY IMPAIRED INDIVIDUALS

#### Braxton Dubin and Michele Williams

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Today, navigation for people with visual impairments in new environments is quite challenging. People with vision impairments navigate environments using orientation and mobility techniques and certain assistive devices. Orientation and mobility techniques include finding where a person is in space and finding the way from that location to a destination. Navigation aids such as a cane, a seeing-eye dog, and sometimes assistive technology are also utilized along with O&M techniques. Navigation is still difficult, however, as many aspects of the environment are purely visual (such as signage) or difficult to identify before reaching it (such as stairs). To test if identifying certain architectural details or other building features could help improve independent navigation, we tested a prototype of an assistive navigation device. The device identifies escalators, stairs, emergency exits, and store logos as the blind participant passes them. Since this is an exploratory study, we used a Wizard of Oz research method where the capabilities of such a device are simulated using an app on an IPad with a set of commands specific to the new environment. Although this is a Wizard of Oz study, the reactions and behavior of the blind participants are a great approximation of their behavior with a real device. During the study with ten participants, we found that additional architectural information was very helpful to people with vision impairments. The device gave information that they wouldn't be able to readily access which supplemented their O&M techniques. Future work will be to continue refining the interface and backend recognition technology based on what the participants found helpful.

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# EFFECT OF *mpkA* DELETION ON CELL WALL INTEGRITY OF *A. nidulans* UNDER MICAFUNGIN AND SHEAR STRESS PERTUBATION

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In the model fungus *Aspergillus nidulans*, the MpkA protein has been identified as a crucial component in the cell-wall integrity signaling (CWIS) pathway, responding to cell wall stress to mediate necessary repairs. It was previously shown deletion of the *mpkA* gene does not allow the cell wall to regenerate after perturbation. The objective of this study was to characterize the effect of the *mpkA* deletion by observing the morphology of the deletion mutant under various perturbation agents. As a control, the deletion mutant was grown in stationary culture, in the absence of any stress (i.e., in liquid growth medium, on cover slips). The mutant was then grown under similar conditions in the presence of the cell wall perturbation agent micafungin (i.e., a beta-glucan synthase inhibitor). The deletion mutant was also grown in a mechanically agitated fermenter, at different impeller speeds, to observe the effects of shear stress on cell wall integrity. In all cases, morphology was observed using optical microscopy and quantified (via ImageJ) to determine the average projected area of the mycelia at various time points during exposure to stress conditions. Micafungin perturbation led to a 25% reduction in growth rate compared to the control. Shear stress studies are in progress.

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# EFFECTS OF A CHROMATIN REMODELER ON MIGRATORY CELL FATE DETERMINATION

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Cell migration is a critical process in the normal development and functioning of organisms in capacities such as wound healing, tissue formation, and immune response. To understand better the mechanisms that determine cells to be migratory or static, we examine collective cell migration in the ovarian tissue of the organism *Drosophila melanogaster*. During egg development in Drosophila, a small subset of somatic epithelial cells are specified as "border cells" which form a cluster and migrate from the anterior pole of the egg chamber toward the oocyte. The highly conserved Janus Kinase/Signal Transducer Activator of Transcription pathway (JAK/STAT) regulates this process, and two downstream targets of the transcription factor STAT, *apontic (apt)* and *slow border cells (slbo)*, are crucial in determining border cell fate.

Previous work has shown that Brahma, a chromatin remodeler affecting availability of DNA for transcription, has an effect on border cell migration through interaction with the JAK/STAT cascade, but its role is still unclear. To investigate Brahma's function, we conducted a series of genetic experiments comparing the migratory phenotypes of *brahma* mutants to controls. Further, to discover genetic interactions between *brahma* and *apt* or *slbo*, we utilized RNA interference (RNAi) to knockdown Brahma in conjunction with each of them and observed the effect on cluster migration.

To simulate Brahma's role in this genetic circuit mathematically, we used an existing model of differential equations representing this pathway that reflects the static versus motile bistability of the system. Into this we introduced a parameter for Brahma, and through bifurcation analysis and a numerical simulation, have shown the effect of Brahma on the system under the assumptions indicated by our experimental results. This work should help further understanding of the impact of chromatin remodeling on the pathways regulating collective cell migration across organisms at large.

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#### HIV ASSOCIATED B-CELL NON -HODGKIN'S LYMPHOMA IN TRANSGENIC MICE

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B – cell non-Hodgkin's lymphoma occurs in about 5-10% of HIV patients. The risk for developing lymphoma is increased 150 to 250 fold for patients infected with HIV as opposed to non-HIV patients. It is believed that B – cell Lymphoma arises when there is an overstimulation of B cells; eventually leading to a lymphoma and possibly metastasis. The exact involvement and pathogenesis of HIV in HIV-associated lymphoma is currently unknown. The HIV transgenic (Tg 26) mouse is a unique animal model for studying certain HIV-associated diseases. The mouse expresses several HIV proteins such as nef, tat, and gp120. It also has a functional deletion of the gag-pol region, which is responsible for transmission of the virus. These mice develop skin lesions as a result of the transgene. B - cell lymphoma arises in about 30% of the Tg 26 mice . Consequently, mice with lymphoma develop lymphadenopathy, splenomegaly, CNS disease, and they have a high lymphocyte count in the blood. These symptoms are comparable to humans. In addition, there are high levels of HIV proteins in affected organs such as the spleen. The observed lymphadenopathy and levels of HIV proteins lead us to believe that HIV plays a role in the over stimulation and activation of B – cells. The lymphoma probably develops due to chronic irritation of the immune system. We are currently trying to figure out where the overstimulation of B-cells originates? We have recently inducing lymphoma in a nude mouse after injecting it with cells from the bone marrow of a Tg 26 mouse with lymphoma. This leads us to believe that the lymphoma may originate in the bone marrow. Further research should be done to investigate the involvement of specific HIV proteins in the development of B - cell lymphoma.

I would like to thank Dr. J. Bryant for allowing me to work in his lab and the Howard Hughes Medical Institute for funding me.

THE ROLE OF CALCIUM IN METABOLIC OSCILLATIONS OF PANCREATIC BETA CELLS REU Site: Interdisciplinary Program in High Performance Computing <u>George Eskandar<sup>1</sup>, Jennifer Houser<sup>2</sup>, Ellen Prochaska<sup>3</sup>, Jessica Wojtkiewicz<sup>4</sup>,</u> Graduate assistant: Teresa Lebair<sup>5</sup>, Faculty mentor: Bradford E. Peercy<sup>5</sup>, Clients: Margaret Watts<sup>6</sup> and Arthur Sherman<sup>6</sup> <sup>1</sup>Department of Computer Science and Electrical Engineering, UMBC <sup>2</sup>Department of Mathematics, East Tennessee State University <sup>3</sup>Department of Mathematics, Creighton University <sup>4</sup>Department of Mathematics, Louisiana State University <sup>5</sup>Department of Mathematics and Statistics, UMBC <sup>6</sup>Laboratory of Biological Modeling, National Institutes of Health

In order to further understand diabetes mellitus, it is necessary to investigate the dynamics of insulin secretion in the bloodstream. Diabetes is a disease characterized by improper concentrations of blood glucose due to irregular insulin production. Beta cells are responsible for the production and regulation of insulin based on changes in glucose levels. Clusters of these cells, known as islets of Langerhans, are part of the endocrine system in the pancreas. Ultimately, insulin secretion occurs because of changes in the calcium concentration levels in beta cells. This dynamical process is composed of electrical, metabolic, and mitochondrial components that work together to release insulin into the blood. A mathematical model has been developed that captures the full dynamics of insulin secretion including the fast- and slow-bursting behavior from electrical and glycolytic oscillations, respectively.

Using the Dual Oscillator Model, we will examine how calcium handling within individual pancreatic beta cells affects the synchronization of metabolic oscillations within electrically coupled islets. Calcium permeability was implemented into the Dual Oscillator Model, and numerical solutions of the system were obtained via Matlab using a modified ordinary differential equation solver for stiff systems and the Automatic Differentiation for Matlab software. A synchronization index has been developed to quantitatively describe the synchronization of variables between nearest neighboring cells and throughout the islet as a whole. We consider how calcium diffusion between heterogeneous cells affects the behavior of metabolic oscillations and their synchronization. In particular, we want to examine fructose-1, 6bisphosphate and glucose-6-phosphate. Our research will show whether calcium diffusion between cells enhances, diminishes, or terminates metabolic oscillations.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author George Eskandar was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Teresa Lebair was supported during Summer 2015 by UMBC.

#### DETERMINING THE STRUCTURE OF THE REV RESPONSE ELEMENT IN HIV-1

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The Rev Response Element (RRE) is a noncoding portion of the HIV-1 genome found on unspliced and singly-spliced transcripts. The accessory protein Rev interacts with the RRE, facilitating nuclear export of these RNAs. Our research focuses on solving the secondary, and eventually tertiary, structure of the RRE using nuclear magnetic resonance (NMR).

Large RNAs such as the RRE (233 nucleotides) are particularly difficult to analyze by NMR due to broad signals and overlapping peaks. The strategy we used to overcome this challenge involved making smaller fragments based on various computational predictions of the full length RRE secondary structure. The comparison of the fragments and full-length spectra can inform us on the presence or absence of these fragments in the structure. With this strategy, we detected a number of elements consistent with the lowest energy secondary structure prediction. To investigate more complicated regions of the RRE, we designed a segmentation strategy in which we split the RRE at one of our confirmed stem loops, which was replaced by complementary base pairs. By independently transcribing these segments, different labeling schemes can be applied to each before they are annealed back together. These differentially-labeled samples assist with the assignment of chemical shifts and distance constraints by enabling precise editing of our NMR spectra.

We will use these assignments to aid further characterization of the RRE structure, providing insight into the details of retroviral RNA nuclear export, thus potentially advancing the development of therapeutics targeting this stage of the HIV-1 life cycle.

We would like to acknowledge the NIH/NIGMS #P50GM103297, as well as the Howard Hughes Medical Institute and Dr. Summers for the opportunity to participate in advancing scientific research.

#### EXAMINING PLANETARY BOUNDARY LAYER HEIGHTS USING CEILOMETERS

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The planetary boundary layer (PBL) is the lowest part of the troposphere where the wind is influenced by the friction of the planetary surface. During the day and in the heart of the warmer seasons, PBL levels tend to have a higher thickness due to the fact that wind speeds and the thickness of the air corresponds with higher temperatures [Haby n.d.]. While the summer days are getting warmer, there is a mixture of aerosols in the air, causing the PBL to expand and become denser throughout the day.

The National Research Council (NRC) [2009] identified lower tropospheric profiling of trace gases, aerosol and thermodynamic quantities as a cross-cutting need for air quality, weather, climate, energy and other national priority economic areas. The lowest two kilometers of the atmosphere are only probed infrequently in time and sparsely in the United States. In particular, the 00Z and 12Z launches of radiosondes are particularly ill-posed to obtain planetary boundary layer height (PBLH), mixing, and depth at the peak of the heating cycle in the daytime.

Potential for continuous monitoring of PBL heights with ceilometer is evaluated. The top of the convective mixed layer can be retrieved from ceilometer returns, using aerosols as a tracer, analytically using the covariance wavelet technique (CWT) [Brooks, 2003]. Accurate determination of the PBL height using the CWT will allow improved weather and air quality.

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# ASSESSING DECADAL CLIMATE IMPACTS ON WATER RESOURCES WITHIN MISSOURI RIVER SUB-BASINS

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It is well documented that decadal climate variability (DCV) has a significant impact on water resources in the Missouri River Basin (MRB). This project aims to utilize multi-decadal simulations of Global Climate Models (GCM) from the Climate Model Inter-comparison Project (CMIP5) to assess the DCV impact on water yield and streamflow over the MRB using a widely utilized hydrology and crop model known as the Soil and Water Assessment Tool (SWAT).

We use low-resolution (~100km x 100km) data from MIROC5 and HadCM3 GCMs with 57 years of climate simulations at approximately 30,000 locations. The weather parameters included in the GCMs are monthly precipitation, maximum/minimum temperatures, sea-level pressure, relative humidity, and surface wind speed. We downscale all the parameters to match high resolution (12km x 12km) observed data using a two-step procedure. First, an interpolation method is utilized to fill in values at locations where the weather parameters are not available, and then multiple linear regression (MLR) is used to capture features of the observed data at the higher resolution. The coefficients from regression are combined with hindcast data from the two GCMs to compute monthly predictions of maximum/minimum temperatures, and precipitation to input into SWAT. A Weather Generator tool in SWAT is used to generate the daily values necessary to input into SWAT from predictions and observed weather statistics.

We modified a previously developed Graphical User Interface (GUI) in R to streamline the process and include more options for users. We explore if the use of different GCMs and the addition of MLR improves the accuracy of predicting the above-mentioned variables in the MRB. The procedures and GUI developed in this project will allow the client to conduct numerous studies with improved efficiency to assess sensitivity of water resources within the MRB resulting from climate variability and change scenarios.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2015. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS–0821258 and CNS– 1228778) and the SCREMS program (grant no. DMS–0821311), with additional substantial support from UMBC. Co-author Kwame Owusu-Boaitey was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Sai K. Popuri was supported during Summer 2015 by UMBC.

# FLUOROQUIOLONE RESISTANT BACTERIA AND GENES DISTRIBUTION IN MARYLAND-BASED WASTEWATER TREATMENT PLANT AND SURFACE WATER

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Fluoroquinolone (FQ) antibiotics are one of the most popular classes of antibiotics which have been intensively used in both human and animals. After consumption, a certain fraction (e.g., ~50% for ofloxacin or ~100% for ciprofloxacin) of FQ antibiotics will be excreted unchanged. As a result, FQ antibiotics have been consistently found in municipal wastewater. Trace concentrations of these antibiotics in wastewater may contribute to the development and spread of antimicrobial resistance. The objective of this work was to simultaneously monitor antibiotic concentrations, antibiotic resistant bacteria (ARB), and antimicrobial resistance genes (ARGs) in wastewater and wastewater-impacted surface water. We hypothesized that fluoroquinolone concentrations can be correlated with the presence of ARB and ARGs in water samples. To test this hypothesis, water samples were collected from various locations in a Maryland-based wastewater treatment plant, as well as surface water from upstream and downstream of the wastewater effluent discharge site. Water samples were analyzed for 15 fluoroquinolone antibiotics using online solid-phase extraction liquid chromatography tandem mass spectrometry with limits of detection around 10 ng/L. The total fluoroquinolone mass concentration ranged from 27 ng/L in upstream surface water samples to 2090 ng/L in raw wastewater samples. Fluoroquinolone-resistant bacteria were isolated on agar plates containing ciprofloxacin, and multidrug-resistant bacteria were selected using extended spectrum βlactamase (ESBL) plates. To verify the presence of fluoroquinolone-resistance genes (i.e., qnrA, qnrB, qnrC, qnrD, and qnrS), polymerase chain reaction and gel electrophoresis techniques were employed. Fluoroquinolone antibiotics and resistance genes were detected concurrently, suggesting that the presence of antibiotics in wastewater and surface water affects the microbial community. Downstream surface water contained higher FQ and ARB concentrations, confirming concerns over the discharge of antibiotic resistance from wastewater treatment plants.

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#### MICROWAVE LYSING AND FRAGMENTATION OF LISTERIA

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The isolation of DNA from bacterial cells has historically been a time-consuming and expensive process. Given the usefulness of microwaves in heating biological systems, a microwave-based process for the isolation of DNA has proven beneficial in terms of cost and speed. Here we describe approaches for the rapid isolation of DNA using a traditional microwave. The use of geometric gold triangles can assist to focus microwaves and thus lyse the bacterial cells and fragment the released DNA. The long term goal of this project is to lyse, fragment, and detect listeria using a rapid and sensitive method known as Microwave-Accelerated Metal-Enhanced Fluorescence (MAMEF). MAMEF is a faster and cheaper method for the detection of microbial pathogens than traditional molecular methods such as polymerase chain reaction (PCR).

## IDENTIFICATION OF POSSIBLE DEMETHYLASES FOR H4 LYSINE 5 METHYLATION IN SACCHAROMYCES CEREVISIAE

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Histone methylation is a post-translational modification system, which occurs on the side chains of lysine and arginine and is most prominent in histones H3 and H4. This epigenetic mechanism has been shown to regulate chromatin structure and has also been linked to several human pathologies such as cancer, diabetes, autoimmune and neurodegenerative disorders. It has also been discovered that histone methylation is a dynamic process that is indeed reversible resulting in histone demethylation. This study is an attempt to identify possible demethylases for lysine residues 5, 8, and 12 in histone H4, which are associated with repression of gene expression in silent genomic regions. To identify the demethylase, we examined the methylation patterns of five strains lacking the demethylases: Jhd1, Jhd2, Ecm5, Gis1, and Rph1.

We deleted each of these genes in a wild type yeast strain generated using homologous recombination. Nuclei were extracted from each of these strains and subject to Western blot analysis with antibodies against histones H3, H4 and H4 K5 methylation.

We will present the western blot results showing enrichment of histones H3 and H4 in our nuclear extracts, and potential signal for H4K5 methylation. This procedure will be followed by a Mass Spectroscopy analysis in order to observe a change in methylation in the ascertained demethylase mutant.

This research should provide evidence of the regulation mechanism of the methylation of lysine residues 5, 8, and 12 on histone H4 which have yet to be characterized.

This investigation was supported <in part> by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences.

# CRYSTALLIZATION OF THE RIBONUCLEOPROTEIN COMPLEX THAT NUCLEATES VIRAL ASSEMBLY

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Human immunodeficiency virus (HIV) is a retrovirus that is responsible for about two million deaths globally each year. Although treatment regimens target various phases of the viral life cycle, increasing instances of drug resistance require the development of new drugs and identification of new drug targets. Viral RNA elements residing in the conserved 5' leader of the HIV-1 genome direct packaging and are recognized by the nucleocapsid (NC) domains of the viral Gag polyprotein. Previous work from our lab identified a 155-nucleotide region in the 5' leader, the Core Encapsidation Signal ( $\Psi^{CES}$ ) that directs genome recognition and packaging. Our goal is to determine the tertiary structure of the  $\Psi^{CES}$  and NC-bound  $\Psi^{CES}$  complex through X-ray diffraction.

The structural flexibility and conformational heterogeneity of  $\Psi^{CES}$  is a potential impediment to obtaining suitable crystals for X-ray diffraction studies. Therefore, two approaches aimed at stabilizing the structure of  $\Psi^{CES}$  were applied. First, a pair of mismatched stacked pyrimidines in the native  $\Psi^{CES}$  serves as a flexible hinge for the extended Dimerization Initiation Site (DIS) hairpin. A canonical pair of mutations was introduced at that site to reduce flexibility of the DIS arm. Second,  $\Psi^{CES}$  binds eight NC proteins with high affinity. NC binding to  $\Psi^{CES}$  may increase the likelihood of crystallization by reducing flexibility. Native and mutated  $\Psi^{CES}$  constructs will each be crystallized with and without NC proteins. The X-ray diffractionderived tertiary structure of the  $\Psi^{CES}$ , particularly in complex with NC, will be crucial in understanding the molecular function and mechanism of HIV-1 genome recognition and packaging, driving the development of targeted therapies.

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### THE OVEREXPRESSION OF CHLOROPLAST CARBONIC ANHYDRASES CAH3 AND CAH6 IN CHLAMYDOMONAS REINHARDTII TO IMPROVE GROWTH FOR BIOFUEL PRODUCTION

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Microalgae grown under the right conditions can produce significant biomass, which can be converted to biofuel and provide an alternative energy solution as a renewable fuel. Many efforts are underway to discover how algae can be grown more efficiently to reduce the cost of algal biofuels. The objective of this project is to learn how to improve the growth of the model green alga Chlamydomonas reinhardtii. This species was chosen because its complete genome sequence is known and it is easy to manipulate, and what is learned about its biology should be applicable to industrial production algal species. C. reinhardtii and other algae rely on CO<sub>2</sub> concentrating mechanisms (CCMs) to elevate the concentration of CO<sub>2</sub> near the enzyme rubisco. A key component of the CCM are carbonic anhydrases (CAs), which catalyze the interconversion of  $CO_2$  and  $HCO_3$ . In this project, we are attempting to overexpress two chloroplast carbonic anhydrases genes, CAH3 and CAH6, which are believed to play a key role in the CCM. CAH6 is found in the chloroplast stroma while CAH3 is in the thylakoid lumen in close proximity to rubisco, the enzyme responsible for CO<sub>2</sub> fixation. CAH3 and CAH6 coding regions were gene synthesized then ligated into a nuclear expression vector. The CAH6 construct was transformed into two different C. reinhardtii strains, CC48 and CC4350. Several lines of transformed cells were cultured and extracts were prepared for western blot analysis to determine which accumulate high levels of protein. We will perform growth curve analysis of the highest CAH6 producers to determine the effect of CAH6 overexpression on growth rate and biomass production.

These results were obtained as part of the Research Experience and Mentoring (REM) program in the Department of Biological Sciences at the UMBC. This program is funded by a grant (REM supplement to NSF-EFRI-1332344) from the National Science Foundation (NSF) Directorate for Engineering (ENG) Office of Emerging Frontiers in Research and Innovation (EFRI).

#### CHARACTERIZATION OF THE HIV-1 5' UTR DIMERIZATION MECHANISM

### <u>Justin Leonel C. Santos, Carly A. Sciandra</u>, Sarah C. Keane, and Michael F. Summers Department of Chemistry and Biochemistry, Howard Hughes Medical Institute, UMBC, 1000 Hilltop Circle, Baltimore, MD 21052

Human immunodeficiency virus type-1 (HIV-1) is responsible for a pandemic that affects roughly 35 million people worldwide. There is no known cure and antiretroviral medications only serve to reduce the progression of the disease. Current treatments target four stages of the viral life cycle: entry, reverse transcription, integration, and maturation. There is currently no treatment that targets the genome recognition and packaging phase of the viral life cycle. HIV-1 selectively packages the dimeric, unspliced RNA genome. Our group is attempting to understand the structural mechanism behind HIV-1 packaging selectivity. Evidence shows that dimerization of the HIV-1 genome is initiated by a palindromic GCGCGC sequence at the Dimerization Initiation Site (DIS) in the 5' leader (5'-L) between two strands of unspliced RNA. However, previous studies in our lab have shown that the 5' L dimer exhibits a more extensive intermolecular interface. We will employ NMR spectroscopy using a mutagenesis strategy known as long-range probing by Adenosine Interaction Detection (lr-AID) in order to further characterize this mechanism as a function of time. RNA samples will be prepared with specific deuterium labeling in order to probe the dimer conformation at different time intervals. At short time intervals we hypothesize that the HIV-1 5'-L dimerization to transition from a "kissing" loop interaction into a more extensive intermolecular dimer interface. Furthermore, we aim to utilize these results into the development of new therapies that target genome selection for packaging.

This research was funded by NIH/NIGMS grant *1P50GM103297* and NIGMS MARC USTAR grant *T34GM00866*, and was conducted at the Howard Hughes Medical Institute at UMBC with support from the Summer Biomedical Training Program (SBTP). Supported in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. We would also like to thank our research team Gregory Carter, Alyssa Florwick, Briaunna Minor, Heather Frank, Dianne Omire-Mayor, and Mian Khalid for their assistance.

### OPTIMIZATION OF LUTEIN YIELD IN CHLORELLA VULGARIS BASED ON CO<sub>2</sub> CONCENTRATION

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Due to the ability to accumulate biomass rapidly through photosynthesis, microalgae have become very useful for production of nutritional supplements like lutein, which can help prevent and slow the progression of cataracts. Microalgal oils can also be extracted to make biofuels for cars and more pertinent to the immediate goal of this project, microalgae are a sustainable food source for fish grown at commercial scale. The primary objectives of this study are to determine which level of carbon dioxide is optimal for algal growth, and the amount of lutein and total cell protein yielded by *Chlorella vulgaris* when cultured with different  $CO_2$ levels. The different  $CO_2$  conditions in this experiment are 0.04% (atmospheric), 5%, and 10%. For the trials testing 0.04% and 5%  $CO_2$  conditions, we detected significantly greater biomass and growth rate with 5%  $CO_2$ . We are monitoring the amount of lutein and protein yielded under each condition and these will be reported. Eventually our results will be used to determine which of the three  $CO_2$  conditions will be used to grow *C. vulgaris* as fish food for *Tilapia sp.* at Baltimore Polytechnic Institute's aquaponics system.

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#### PROTEIN: RNA INTERACTIONS THAT NUCLEATE HIV-1 VIRAL ASSEMBLY

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36 million people are currently infected with human immunodeficiency virus (HIV), a retrovirus responsible for the onset of the acquired immunodeficiency syndrome (AIDS). Upon transmission, the virus invades CD4<sup>+</sup> T cells and integrates its proviral genetic material into the host genome leading to a life-long infection. During the viral life cycle, interactions between the unspliced viral RNA and its translated product, the Gag polyprotein, initiate the packaging of two copies of the HIV genome. Gag contains three structured domains: Matrix (MA), Capsid (CA), and Nucleocapsid (NC). The NC domain of Gag binds to regions of the 5'-leader (5'-L) within the dimeric HIV-1 genome to initiate genome packaging and viral assembly.

We seek to characterize the Gag-RNA interactions essential to genome packaging through the use of both mature NC and a truncated Gag derivative, CA-p2-NC (CANC). Capsidcapsid interactions promote the formation of distinct units called hexamers. We hypothesize that the hexameric structure of the CA domain contributes to dimeric RNA genome selection. However, hexamer-hexamer interactions in the C-terminal Domain (CTD) of CA lead to protein aggregation and precipitation in the presence of RNA. To circumvent these problems we have introduced W184A and M185A mutations into the CTD of the CA domain of CANC. These mutations prevent the CTD interactions that cause dimerization among hexamers. With these three protein constructs, we aim to deduce the qualitative conditions and thermodynamic parameters of these Gag-RNA interactions using electrophoretic mobility shift assays (EMSA) and isothermal titration calorimetry (ITC).

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