Purdue Physics REU 2017
Final presentations

Thursday August 3, 2017, ROOM PHYS 242

9:00 Julia Spina (prof. Savikhin, prof. Slipchenko)
9:20 Curtis Peterson (prof. Mugler)
9:40 Jonah Quirk (prof. Elliott)
10:00 John W. Scott (prof. Chen)

10:20 – 10:30 *break*

10:30 Samuel Studebaker (prof. Lang)
10:50 Mikael Toye (prof. Pyrak-Nolte)
10:10 Emma Dawson (prof. Iyer-Biswas)
10:30 Daniel Orth (prof. Hung)

11:50 - 1:20 *Lunch (on your own)*

1:20 Jeremy Hartse, (prof. Malis)
1:40 Morgan Heckman, (prof. Pushkar)
2:00 Jesse McDonald (prof. Jung)
2:20 Daniel Murphy (prof. Kais)
2:40 Kim, Sang Woo (prof. Lang)*

3:00 *The end*

*Not funded by REU NSF grant

6:30 - *Farewell party/picnic at Sergei Savikhin's house for REU students, advisors, speakers & significant others*
Address: 2505 McShay Dr., West Lafayette
Phone: 765-413-5026 (cell)

Modeling Photosynthetic Fenna-Matthews-Olson Complex (FMO)

Julia Spina, Valentyn Stadnytskyi, Yongbin Kim, Zachary Mitchell, Sergei Savikhin, Lyudmila Slipchenko

Photosynthesis is the process by which organisms efficiently convert photonic energy, CO2, and an electron donor into chemical energy. Studying the excitonic structure of certain photosynthetic systems allows us to better understand photosynthesis and thus improve models for artificial photosynthesis and energy transfer networks. One such photosynthetic system is the Fenna-Matthews-Olson (FMO) complex, a trimer present in green sulfur bacteria that mediates the transfer of photonic energy during photosynthesis. Each monomer contains 7 pigments (with an 8^{th} pigment located in the center of the trimer) that absorb and transfer the photonic energy throughout the complex via resonant energy transfer. Each monomer can be modeled quantum mechanically as an 8x8 Hamiltonian written in the basis of wave functions for the different pigments, where the energies along the diagonal are the excitation energies of the pigments and the off-diagonal elements represent weak dipole-dipole interaction potentials. It is ambiguous what single Hamiltonian described FMO since many feasible models have been suggested that fit existing experimental data, and this uncertainty can be addressed with experimental and computational methods. Possible Hamiltonians can be extracted from the room temperature, steady-state absorption spectrum of the FMO complex, but there are certain shortcomings with this method of generating the excitonic model. There are an infinite number of composite Gaussian distributions that fit the FMO absorption spectrum; experimental factors have been used to narrow down the feasible number of Hamiltonians to 10, but it is not clear which one of the 10 is truly correct. Additionally, the 8 pigments are close to each other and electrostatically coupled, making it difficult to determine the individual contribution of each pigment to the absorption spectrum of FMO. This fact raises questions about whether the diagonal entries in existing Hamiltonian models were assigned correctly. Finally, the pigments, being electrostatically charged structures, have transition dipole moments and are thus sensitive to the polarization of light used to measure the absorption of FMO. Since absorption spectroscopy uses unpolarized light, there is likely important excitonic structural information that is not obvious when using absorption spectroscopy alone.

These concerns with the accuracy of current models were experimentally substantiated by a series of later experiments involving the ultra-fast time-resolved CD spectroscopy of mutated FMO complexes. With femto-second time resolution, it is possible to precisely observe how the spectrum of FMO evolves with time, as opposed to exclusively looking at the steady-state spectrum. Additionally, by mutating the amino acid structure of the protein complex around each pigment, it is possible to suppress the function of individual pigments and get a better idea of how each pigment contributes to the absorption spectrum of FMO. Finally, measuring the spectrum of FMO with circularly polarized light (CD spectroscopy) instead of unpolarized is more sensitive to the relative orientation of the transition dipole moments of each pigment, and thus yields more structural information about the FMO complex than absorption spectroscopy alone. This series of experiments demonstrated that certain pigments do not fit any theoretical models well, differences that are not as apparent in when using absorption spectroscopy. These results suggest that values in the Hamiltonians for FMO have been misassigned at some

point, and provides motivation for my own experimental project. The objective of my experimental project is to determine the time resolved CD spectra of wild FMO complexes at 77K use and these results to improve the accuracy of existing photosynthetic models. Cooling the sample makes the peaks in the absorption spectrum sharper and more defined, indicating the distinct energy bands of the different pigments. Preliminary analyses indicate that CD decay behavior is present when measuring the CD spectrum of cooled mutated FMO complexes, as it was when measuring the sample at room temperature. Further analysis is necessary to generate the full CD spectrum of mutated FMO at 77K.

In addition to this experimental project, I have also been working on a similar computational project. The goal of this project is to determine the shift in the room temperature absorption spectrum of FMO that results from mutating pigment #4. The crystal structure of the FMO trimer was determined decades ago using X-ray crystallography, and by hardcoding the amino acid mutation associated with pigment #4, it is possible to computationally determine the resulting shift in the absorption spectrum. After generating the classical vibrational modes of the mutated structure over 40ns, a clustering analysis based on the RMSD values of the trajectories yielded the most probable structures. Those structures were then submitted for quantum computations, where quantum dynamics simulations were run on segments of interest and the surrounding environment was treated classically. More specifically, the quantum computations run on the most likely trajectories were QM/MM, a computation technique that treats electrostatically charged structures as point charges and analyzes interactions between the quantum and classical regions with classical electrodynamics. The shift calculated was 156.18cm-1, which is a surprising result because preliminary computational results suggest that pigment #4 should become the lowest energy pigment after mutation and have a much smaller associated shift than this.

I would like to thank the Purdue University Physics Department for offering me the opportunity to participate in this REU. I would also like to thank Professors Sergei Savikhin and Lyudmila Slipchenko for hosting me in their groups and Valentyn Stadnytskyi, Yongbin Kim, and Zachary Mitchell for training and guiding me during this REU. I would finally like to thank the NSF for providing the REU grant PHY-1460899, which supported my employment.

Critical Dynamics of Biochemical Systems

Curtis Peterson[1,2]*, Tommy Byrd*[2]*, Amir Erez*[3]*, Andrew Mugler*[2]
[1]Department of Physics, Arizona State University, [2]Department of Physics and Astronomy, Purdue University, [3]National Cancer Institute, National Institutes of Health

Cell behaviors are governed by non-equilibrium systems of interacting molecules. Often, these systems exhibit qualitative transitions in their parameter space, e.g. from one to two stable states. These transitions are reminiscent of phase transitions in equilibrium systems from many-body physics. Indeed, a particular class of non-equilibrium biochemical systems has been shown to exhibit the critical scaling properties of the Ising universality class in the mean-field limit, and this prediction is supported by measurements of doubly phosphorylated ppERK in T cells [1]. These systems, however, have only been studied in steady state. The goal of my project has been to extend this analysis by studying these systems as they are driven out of steady state via a quenching process, utilizing both the biochemical feedback model of [1] and experimental data from T cells.

Experimentally, the quenching process is caused by exposure of cells to varying doses of an enzyme-inhibiting drug. In response to the drug, the distribution of ppERK molecules undergoes a large shift over time for large drug doses (Fig. 1A), or a small shift over time for small drug doses (Fig. 1B). Following [1], the initial and final states of these distributions correspond, in the language of the Ising universality class, to particular values of an effective magnetic field h and an effective reduced temperature θ (Fig. 1C). Our hypothesis is that distributions that are driven closer to the critical point ($h = \theta = 0$) will take longer to relax to their final state due to the phenomenon of critical slowing down. I tested this hypothesis by extracting the relaxation time from a divergence measure between the time-dependent distributions and the final distribution, and plotting

it against distance from the critical point (Fig. 1D). The existence of a downward trend in Fig. 1D indicates preliminary evidence for critical slowing down in T cells.

Future work will investigate the analog of Fig. 1D using the biochemical feedback model of [1]. We expect that we will also see a downward trend, which will provide an explanation for our experimental observations in terms of critical slowing down. I have already begun this investigation, and my coauthors will continue this work in consultation with me going forward.

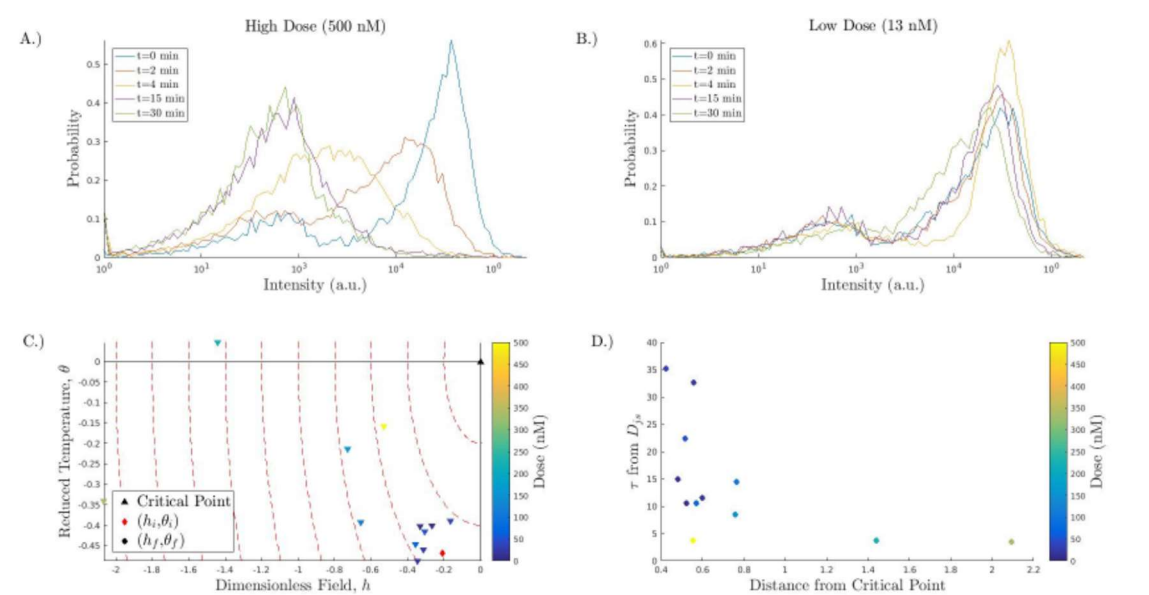


Figure 1. (A,B) Dynamics of ppERK distribution in T cells in response to drug (C, D) and mapping to effective parameters of the Ising universality class.

This work was supported by NSF REU grant PHY-1460899.

[1] A. Erez, T. A. Byrd, R. M. Vogel, G. Altan-Bonnet, A. Mugler, arXiv:1703.04194.

Lifetime Measurement of the 7s State in Cesium

Purdue University, IN
Jonah Quirk

Accuracy in the interpretation of parity nonconservation experiments in cesium rely on accurate measurements in the lifetime of atomic transitions. Previous experiments have cited results with one percent accuracy. This experiment is aiming for .1 percent accuracy. This difference in accuracy could be obtained from updated techniques, updated equipment, and minimized systematic effects. These systematic effects can arise from quantum beats, radiation trapping, diffusion of atoms out of the detection region, and atom-atom collisions.

The system is set up such that a 1079 nm laser will pass through a laser amplifier to reach a power of 1 W. The laser beam will then pass through a vapor cell to lock the laser to the required transition. The remaining portion of the beam will then pass through an acusto-optic modulator. The main portion of the beam will be sent to a beam dump. The deflected portion will be routed around and into a second vapor cell. The second vapor cell is housed inside of a hollowed aluminum cylinder with 5 mm viewports in the ends of the long axis, and a 1 inch viewport milled to house a 1 inch lens tube. The exterior of the aluminum cylinder is wrapped in heating tape and aluminum foil to adjust the temperature. The AOM will be pulsed on for around 700 ns and off for 300 ns. This will direct the beam through the vapor cell exciting a two photon transition during the 700 ns. This two photon transition will excite an atom from the 6s to 7s state. The atom will then decay to the 6p3/2 and then decay to the 6s, the latter of which is accurately known. A single photon detector will sense the arrival of one photon and record the time accurately. This process will yield a double exponential decay which can be fitted to determine the lifetime for the 7s state.

My contribution to this project included milling of the aluminum cylinder, fabricating a mound for magnetic field coils and general setup of the experiment. I also worked on two Littman lasers, magnetic field coils for two other experiments, and circuit fabrication and debugging.

I would like the thank Dr. Elliott and his entire lab for helping me and allowing me to work in their lab. This work was supported by NSF REU grant PHY-1460899

Raman Spectroscopy of *E. Coli.* in C3D Process

John Scott[1], Jack Chung[2], Dr. Eduardo Ximenes[3], Xingya Liu[4], Brendan Sullivan[2], Dr. Yong Chen[2,4]

[1]Carleton College, Mn

[2]Purdue University Dept. Of Phys. And Astr., IN

[3]Purdue University LORRE, IN

[4]Purdue University Coll. Of Engineering

Food borne illness is a widespread problem in the U.S. and abroad, with millions of individuals affected on a yearly basis while incurring a substantial financial cost from both the human impact as well as the damage done to the economy. Current detection methods, principally polymerase chain reaction-derived methods, do not operate fast enough to control outbreaks of food-borne illness. In a collaboration with Purdue's Laboratory of Renewable Resources Engineering (LORRE), and operating under Discovery Park's Big Ideas Challenge, Dr. Chen's group is working towards using a combination of micro-filtration and photonic methods, known as the C3D, including Raman spectroscopy, to speed the detection of food-borne pathogens.

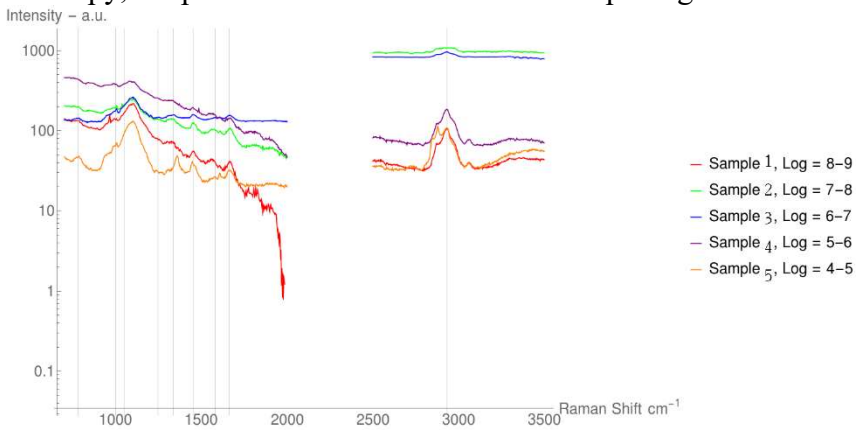


Fig 1.

My objective in this research was to reach an initial operating capability for the Raman spectroscopy of bacteria. This includes determining suitable measurement conditions for the Raman spectroscopy, investigating methods of sample preparation, visually detecting, and suggesting methods for integrating the Raman detection process with the rest of the C3D process. Ultimately the goal of this process was to outline the requirements of the preparation process for Raman detection and to successfully measure Raman spectra (Fig. 1) for bacterial samples with an extremely low target density comparable to that produced by the C3D process. As of current I believe the final method will integrate fluorescence microscopy (Fig. 2) as a method to visually mark the target pathogens for individual identification. This method could be integrated as an automated, encapsulated, component of the C3D process, offering a substantial improvement in terms of detection time over current PCR based methods.

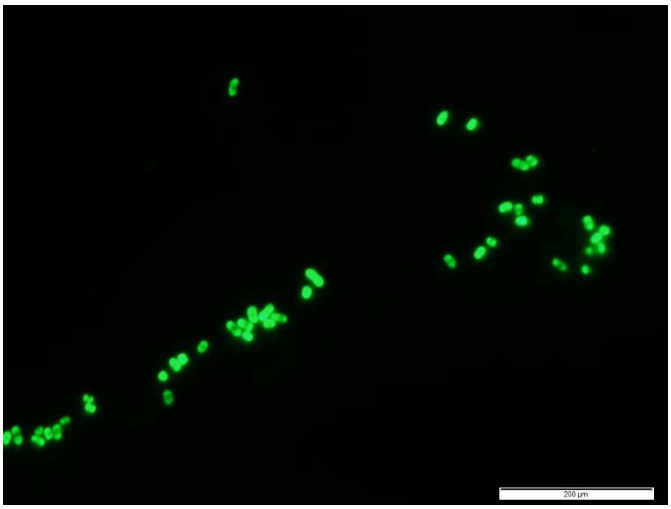


Fig. 2.

I am happy to have been able to work in Purdue's REU program this summer. I would like to thank Jack Chung, Dr. Eduardo Ximenes, Xingya Liu, Brendan Sullivan, Andres Allcca, Nirajan Mandal, and the rest of the QMD Lab and BIC team. I would also like to thank NSF REU grant PHY-1460899 for supporting my work.

XENON1T: The Search for Dark Matter

Samuel Studebaker[1], Darryl Masson[1], Rafael Lang[1]
[1]Purdue University, IN

XENON1T, a dual phase time projection chamber in Italy, is the most sensitive detector in the world. It was designed to detect Weakly Interacting Massive Particles (WIMPs), a dark matter candidate predicted by Supersymmetry. XENON1T is filled with liquid and gaseous xenon that produces photons and electrons during a particle interaction. The photon is detected by PMTs in the detector and is called the S1 signal. The electron is drifted up through an applied electric field and then accelerated into the gaseous xenon, where it produces photons of its own. These photons, the significantly larger S2 signal, are detected by the PMTs after the S1 signal. The depth at which the interaction occurred in the detector can be calculated from the time difference between the two signals.

Although XENON1T was built to detect WIMPs, it can also be used to detect other particle interactions, such as neutrinos. Neutrinos, unlike WIMPs, are low mass particles that only produce a S2 signal because their interaction with the liquid xenon is not energetic enough to produce a detectable S1 signal. Thus, S2-only background events, which were easily filtered out while searching for WIMPs, are now important. S2-only background events are believed to be caused by the photoionization of impurities in the liquid xenon and the photoelectric effect in the detector's metals. These stray electrons do not have enough energy to cross from liquid to gaseous xenon and become trapped. Eventually, they get bumped and receive enough energy to enter the gas and produce a S2 signal. One proposed solution to this problem has been to add infrared LEDs in the detector. These LEDs would provide enough energy for the electrons to cross the barrier, and the infrared light (940 nm) would not be detected by the PMTs.

Here at Purdue University, Professor Rafael Lang and the Dark Matter group have set up Asterix, a smaller version of the XENON1T. Since this detector is scaled down, it can be used to quickly test proposals. Our objective this summer was to get Asterix operational and to add in the necessary components to test out the theory that infrared LEDs would help eliminate S2-only background events. To test this theory, Asterix needed to be disassembled so that an infrared LED could be installed. We also installed infrared photodiodes so that we could confirm that the LED was working inside the detector. Furthermore, we needed a detectable signal from the photodiodes so I designed, assembled, soldered, and tested an amplifier that is now mounted on the detector. Furthermore, all the wiring for the detector components needed to be installed and documented.

This work was supported by NSF REU grant PHY-1460899.

Swarm Flow Through Porous Media

Mikael Toye[1], Alison Hoe[1], Laura Pyrak-Nolte[1]

[1]Purdue University, IN

The use of nano- and micro-particulate material in many industrial application has lead to an increase interest in aqueous particulate transport in the subsurface. A droplets with small dilutions of particles move through an aqueous environment, they undergo hydrodynamic interparticle interactions that gives rise to group behavior, termed swarm behavior. Swarm behavior is further affected by boundary conditions defined by the size, shape, and amount of media a swarm passes through. In particular, swarm transport has been shown to accelerate in fractures, termed enhanced transport. Our goal is to observe microparticle swarms transport across the fracture matrix interface in 3D synthetic porous media to determine the effect of fracture aperture on swarm speed and evolution.

My first objective for this research project was to set up an experimental table to conduct swarm experiments in a 3D transparent porous medium that enabled imaging of the swarm from two orthogonal directions. One camera directly imaged the tank setup, while the second camera used a system of 2 mirrors to capture an orthogonal side view.

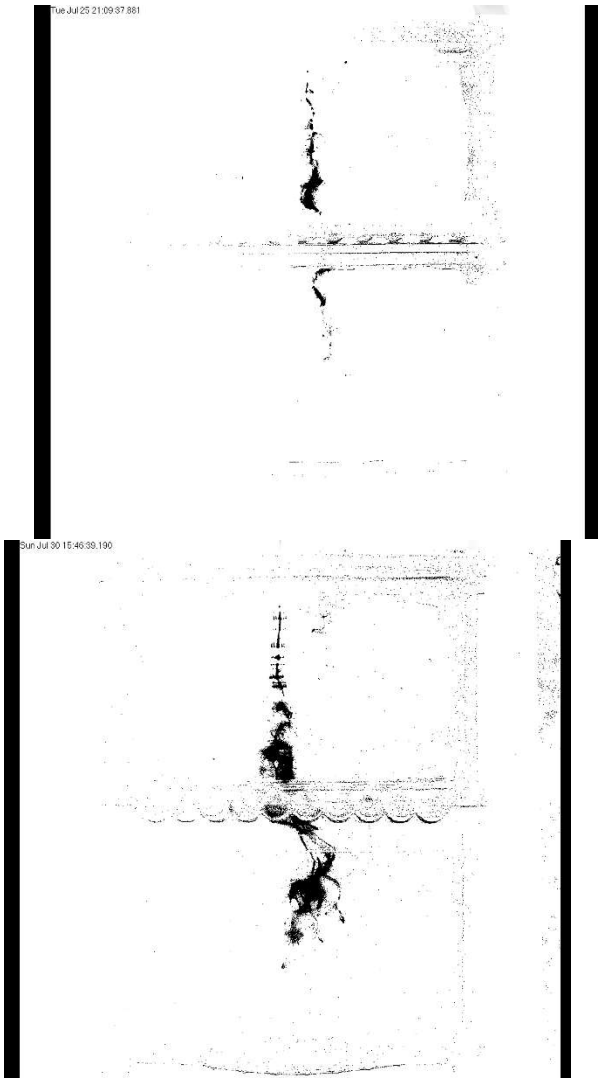
The next task was to design an apparatus to hold a granular porous medium that would allow for uniform swarm behavior and clear imaging. In these experiments, hydrogel spheres were used to create a transparent porous medium. My designed was based on a previous design created by Alison Hoe that featured two stacked prismatic holders stacked. I redesigned the lower surface of the top holder to create a fracture surface that more closely resembled the hydrogel. Using Autodesk Inventor, I drafted the designed and then printed it with a 3D printer. In my design, the top frame of the lower holder was eliminated to enable for better visualization of swarms passing through the aperture and into the lower porous medium. This mitigated any global horizontal flow through the aperture.

After refining the experimental set-up, I conducted 15 and 20 µL swarm experiments with fracture sizes of 10 mm, 1mm, and 0 mm between the porous media holders. The entire experiment was performed in an aqueous solution of 0.0075 g/mL of KCl. The swarms had a density of 1% fluorescent polystyrene beads (approximate diameter 3.2 µm) mixed with 0.015 g/mL of KCl to ensure the swarms sunk at the desired rate. The swarms were released ~10 mm above the upper holder and a 25.4 mm below the surface of the water to avoid surface currents. In general, the swarms took one to two hours to transport through the entire apparatus.

To analyze the images from the swarm experiments, I wrote a MATLAB code to process the frames taken by the two cameras of the swarm experiments to isolate and amplify the visibility of the swarms. Using these edited images, a frame summing technique was used to derive a position and velocity plot of the head of the swarms.

The data analyzed thus far suggests that the swarms tend to have a larger area of spread upon reentry into the porous media after passing through a larger aperture. The experiments with 0 mm apertures typically resulted in swarms continuing down one

path. In contrast, the experiments with the 10 mm aperture showed swarms bifurcating over hydrogel in a cascade like path, usually growing in width in one direction.



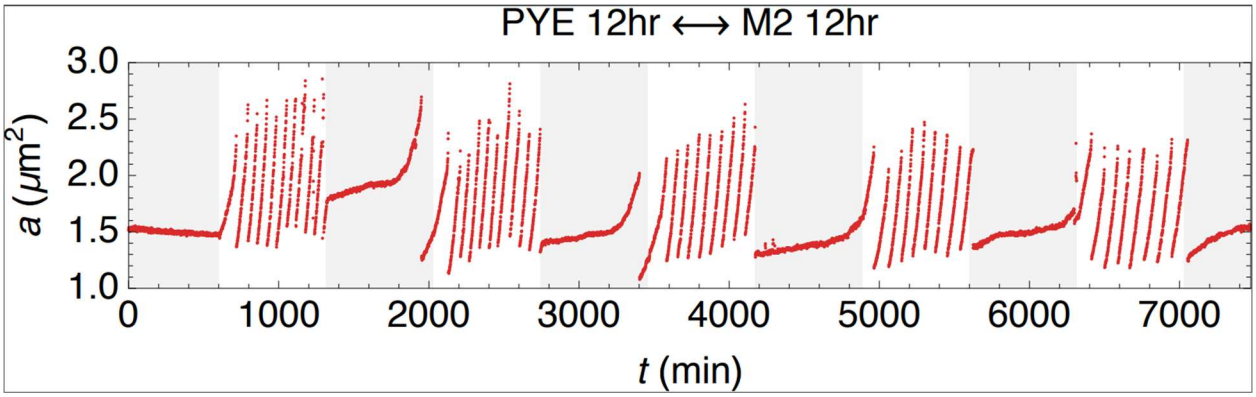
Left: A 15 µL swarm passing through a closed (0 mm) aperture. Right: A 20 µL swarm passing through a 10 mm aperture. *Note: The 20 µL swarm data for small apertures is currently under analysis and thus could not be used in this report.

I am thankful to have been given the opportunity to be a part of Purdue's REU program. I would like to thank professor Laura Pyrak-Nolte for her guidance throughout my research and experiments, as well as Alison Hoe for her previous work with this research. I would also like to thank the U.S. Department of Energy for sponsoring my work (Award Number DE-FG02-09ER16022). This work was also supported by NSF REU grant PHY-1460899.

The Physics of Stochastic Single-Cell Dynamics

Emma Dawson[1,2], Farshid Jafarpour[2] , Srividya Iyer-Biswas[2]
[1]St. Olaf College, MN; [2]Purdue University, IN

Historically, physicists have worked to determine the quantitative laws that govern the dynamics of inanimate matter. We are working similarly to determine the quantitative laws that govern the dynamics of living systems and to solve the unique problems presented in doing so. One barrier in the study of living systems is the exponential growth of cell populations which makes the study of single cells difficult over extended periods of time. A unique optical and biological method has been developed to remove this barrier, allowing for the study of single cells for tens to hundreds of generations. The abundance and density of data this method provides has allowed for the determination of quantitative laws governing cell dynamics. Specifically, I will discuss a recent effort to characterize the scaling laws governing stochastic single-cell aging.



Above: A Caulobacter Crescentus cell grows and divides over 10 successive 12hr periods alternating between M2 (a minimal media in which the cell starves) and PYE (a rich media in
which the cell feeds). The cell shows periods of growth and division during pulses of PYE and dramatically slowed growth during pulses of M2. Here, aging is evident in progressively slower growth and division during pulses of PYE.

This work was supported by NSF REU grant PHY-1460899

Grating Coupler Optimization for Nanophotonic Quantum Simulator

Daniel Orth[1], Tzu-Han Chang[2], Chen-Lung Hung[2]
[1]University of Dallas, TX; [2]Purdue University, IN

Our research group intends to create a system of long-range spin models by coupling laser-cooled atoms to photons in order to induce photon-mediated atom-atom interactions. To create strong atom-photon interactions, we plan to couple atoms to guided mode photons in nanophotonic structures. This requires efficient coupling of photons into and out of a nanophotonic circuit in order to characterize the photonic property of a circuit or to manipulate laser-cooled atoms that are trapped on it.

My project is the optimization of a diffraction grating used to couple light into the waveguide on the aforementioned circuit. To accomplish this, I ran computer simulations of a two-dimensional model of the grating coupler and designed a three-dimensional model for later use. To optimize the grating coupler, I used the Lumerical FDTD Solutions software, which allowed me to create a virtual model of the coupler and run a finite difference time domain (FDTD) simulation of its performance. In my simulations, I ran sweeps over possible values of certain parameters and recorded the fraction of the light that was successfully transmitted. Using these results, I was able to approximately optimize these parameters for maximum transmission. Once I had finished optimizing the two-dimensional model, I created a three-dimensional model of the same structure with the optimized parameters.

I would like to thank the NSF REU grant PHY-1460899 for supporting this project, and I would also like to thank Professor Chen-Lung Hung and Tzu-Han Chang for their guidance throughout the project. I have learned a lot from Purdue's REU program, and I am grateful to have participated.

Photosystem II

Morgan Heckman, Scott Jensen, Dan Hartzler, Yulia Pushkar

Purdue University, IN

The process of photosynthesis has been studied both to understand how the system works, as well as to try and replicate it. If the process of translating energy taken from photons into chemical energy can be recreated outside of plants, then we would have a more efficient and cheaper way to harvest solar energy. This is becoming increasingly necessary as we try to find better ways to utilize our natural resources, and do so in ways that are economically competitive with the government subsidized coal and natural gas markets.

Photosynthesis is a complex process, and for the purpose of my work here, we have focused on the Oxygen Evolving Complex (OEC) within Photosystem II in the light dependent reactions. The OEC is a cluster of atoms, Mn_4CaO_5, that is responsible for taking in the energy from photons and splitting water, releasing oxygen as a byproduct. This breaking of water molecules is essential to the rest of the photosynthetic process. The OEC goes through an S-cycle, which incoming photons help drive.

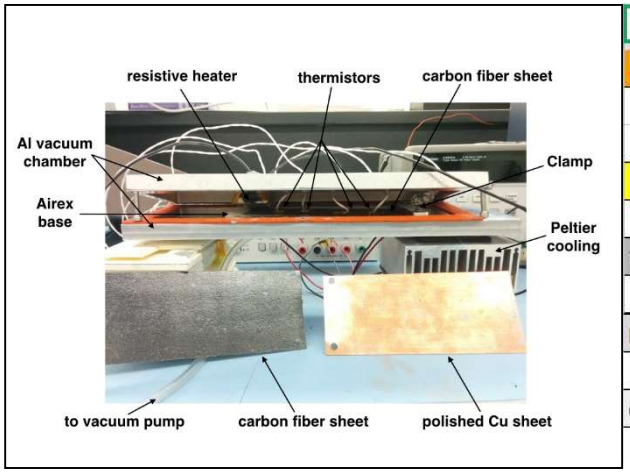
My work has been mainly with the mechanism we use to lay out our sample PSII in order to study the states within the S-cycle. We've been trying to optimize the layout of our system so that it can be used for two separate experiments without having to be dramatically reworked, as time is limited once we are at the beamline in Argonne National Lab to collect data. One of these experiments required the delivery system to be upside down in comparison to the orientation of the other experiment. I have also worked with some of the background reading to determine what needs to be studied, and participated in some of the data collection at Argonne National Lab, in addition to occasionally working on various other projects within the lab.

I would like to give thanks to the Purdue Physics and Astronomy department, and Professor Pushkar's lab especially, for this opportunity. I have been very gratefully to all those who I have been able to work with throughout this summer, especially Scott Jensen who worked with me the most. I would also like to thank the NSF REU grant that has supported my work.

Thermal Conductivity of Carbon Fiber Structures

Jesse McDonald, Branden Burns, George Mitchell, Mihir Kodak,
Andrew Spring, Alexander Wade, Souvik Das, Andreas Jung
Purdue University, IN

Investigations into the physics of fundamental particles at the Large Hadron Collider (LHC) at CERN led to the discovery of the Higgs boson in 2012, the mass particle. In a proposed upgrade to the LHC for 2023, the rate of reactions inside the accelerator will be increased ten fold. To keep up with this increase, the Compact Muon Solenoid experiment will be fitted with customized sensor chips. These chips must be housed in lightweight but highly thermally conductive structures to cool them and avoid radiation damage. This work proposes and explores the use of carbon fiber (CF) with embedded graphite as a novel material for making such structures.



Round 2	Voltage (V)	r (ratio to Cu)
Copper Sheet	10	1
	10	1
	17	1
Carbon Fiber	10	1.502806714
	17	1.365555824
Top Sheet	10	1.04915284
	17	1.23551958
Half Inch	10	1.437256967
	17	1.518869109
Carbon Fiber Perp	10	1.063501384
	17	1.189800095

The thermal conductivity of a material is determined as the ratio of heat flux through it to the temperature gradient across it. We machined our apparatus out of aluminum as a vacuum chamber that holds a sheet of the test material between an electrical heat source and a Peltier cooling element. Four thermistors are placed in a straight line on the sheet between the heat source and the sink to determine the temperature gradient. To calibrate our apparatus, we measure the thermal conductivity of copper. We report ratios of thermal conductivities of test materials to this measurement of copper to mitigate systematic uncertainties from the apparatus.

Measurements of 3 ply CF in different orientations offer us a way to measure thermal conductivities of single plies parallel and perpendicular to the grain. We find that the thermal conductivity of 3 ply CF embedded with graphite is higher than that of copper. We also find that CF with graphite is a marginally better conductor than CF within experimental uncertainties. This leads us to suggest perfecting the co-curing process in future experiments.

I am very thankful to have been a part of the REU program at Purdue. Professor Jung, Souvik Das, and the rest of the research group I have been with this summer have been a tremendous help. This work was supported by NSF REU grant PHY-1460899.

Direct Application of the Hamiltonian in the Phase Estimation Algorithm

Sabre Kais, Teng Bian, Daniel Murphy

Purdue University, IN

Given a unitary operator U we can estimate the angle of a phase it puts on an eigenstate of by applying one of various phase estimation algorithms to this state. Therefore, it is obvious that the ability to easily encode information about hamiltonian eigenvalues in the phase of a Unitary can have huge application over various fields of computational chemistry, physics, and biology. The obvious case is Hamiltonian exponentiation. This produces a unitary with its eigenvalue encoded in the phase. The most common choice for implementing this unitary is the Trotter-Suzuki approximation as it expresses the exponentiated hamiltonian to arbitrary order of accuracy with a series of multi qubit rotations on the state register. The issue with this method is the exponential scaling of gates required, with increase in the size of the hamiltonian. This would become inefficient for simulating hamiltonians of more complex systems. A more direct application of the hamiltonian could only apply XYZ operators to the qubits in the state register and thus decrease the number of gates drastically. Calculating an approximate Unitary directly with the terms of hamiltonian we can implement a phase estimation with significantly less gates, and for a N qubit hamiltonian with L terms this method requires Log(L) + N + 1 qubits. My work these past 10 weeks has so far shown that this method of direct application of the hamiltonian in phase estimation produces data for the ground energy of water molecule which agrees with both diagonalization of the hamiltonian and phase estimation on the exponentiated hamiltonian approximated with the TS series.

Radon Self-Veto in the XENON1T Detector

Sang Woo Kim[1], Darryl Masson[2], Abigail Kopec[2], Dillon Davis[2], Joe Skeens[2], Rafael Lang[2]

[1] University of Notre Dame, [2] Purdue University

Physicists are convinced of dark matter's existence and its properties, but are not sure of what exactly it is. A candidate that arises from many theoretical models is the weakly interacting massive particle, or WIMP, and liquid noble gas detectors have been in the forefront of efforts to directly detect it. The XENON1T detector, located in Gran Sasso, Italy, is the most sensitive among these liquid noble gas detectors. It is located a mile underground and utilizes a dual phase time-projection chamber (TPC); interactions within the TPC produce scintillation photons and ionization electrons that are recorded by photomultiplier tubes below and above the TPC.

The XENON1T detector earns the title of being the most sensitive WIMP detector in the world due to its incredibly low background counts, which is a result of the pureness of the material that comprise it, the pureness of the xenon, and the self-shielding property of xenon. Of the background sources present at low energies, the radon-222 decay chain is the most prominent (Figure 1). Within the decay chain, the lead-214 decay is the culprit; the radon-222 decay and the polonium-218 decays are alpha decays, which makes them easy to tag, and the extremely short half-life of polonium-214 makes the bismuth-214 and the polonium-214 decays (BiPo decay for short) easy to tag as well. Since the lead-214 decays can produce low-energy events that can be confused with WIMP signals, it is of our best interest to remove them as much as possible. In turn, we can even further increase XENON1T's WIMP sensitivty. Dr. Rafael Lang's group at Purdue University has been developing an offline analysis method called radon self-veto to remove this radon-222 decay chain.

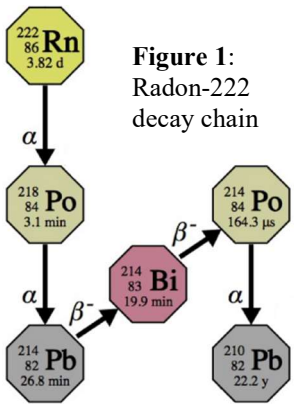


Figure 1: Radon-222 decay chain

Radon self-veto utilizes convection, which is a temperature-driven movement of the liquid xenon within the TPC. If we understand convection well, we should be able to go backwards in convection and time from a BiPo decay to find a lead decay, and go even further back in convection and time to find the polonium decay and the radon decay. Since we do not yet understand convection, however, we start by using a convection-agnostic method: for each BiPo decay, we look for low energy events in all directions by drawing a big sphere around it. We call this the big sphere method, and we find that there is a highly significant number of low energy events in our spheres created around BiPo decays.

In order to move past the big sphere method and increase the effectiveness of radon-self veto, we must understand convection well. We find that we can start to do this by pairing radon-222 decays with polonium-218 decays and creating a velocity vector field which serves as an initial version of a convection map of the liquid xenon. The convection map is not perfect yet, but there are ongoing efforts to improve it. Once we have a good understanding of convection, radon self-veto should be able to find a good majority of lead events that occur at low energies, veto them, and increase XENON1T's WIMP sensitivity to even higher thresholds than ever before.