Please Note: Applicants should **NOT CONTACT FACULTY** during your application phase, which is unfair to other applicants. You may be disqualified for iSURE by doing so. For **ANY** questions, please contact Lisa Shroyer (lshroyer@nd.edu) or Amber Li (zli15@nd.edu).

iSURE 2017 Research Projects

Below is the list of iSURE research projects for summer 2017. In the online application, please select up to three research projects (Question 1) and rank them in order in the text box (Question 32).

Projects Offered for BOTH time frames

(8 week June 4th – July 29th AND 6 weeks July 2nd – August 12th)

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Projects Offered for 8 week timeframe

Center for Research Computing (CRC) REU Program Projects

(8 week June 4th – July 29th)

Note: Only students who will be able to attend the program from June 4th – July 29th can apply to the following projects:

DISC – Data Intensive Scientific Computing

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41. (VIS) Data Visualization…………………………………………………………………..Page 21
42. (CYBER) Distributed Data and Cloud Based Cyber Infrastructure for Science……………………Page 22
43. (DISTSYS) Distributed Systems for Scientific Computing………………………………………...Page 22
44. (BIOMETRICS) Data-Intensive Deep Learning for Biometrics…………………………………....Page 22
45. (NETSCI) Network Science for Computational Biology…………………………………………..Page 22

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46. (LOBSTER) Crunching LHC Data on 25K Cores witLobster……………………………………...Page 23
47. (MDAPP) Modern Data Analytics Approaches in Particle Physics………………………………...Page 23
48. (CLAD) Classification in Large Astrophysical Databases………………………………………….Page 23
49. (EAIG) Exploitation of Astrophysical Imaging within the Galaxy……………………………....Page 23
50. (NMLAP) Novel Machine Learning Approaches in Physics……………………………………….Page 24

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51. (CG) Computational Genomics…………………………………………………………………….Page 24
52. (TRAITS) Identifying Bacteria Ecological Syndromes and Tradeoffs through Comparative Genomics……………………………………………………………………………………...Page 24
53. (HYDRO) Coupled Hydrologic and Biogeochemical Modeling of Lake Regions…………………Page 25
54. (EVGR) Epigenetic Variation and Gene Regulation………………………………………………..Page 25
55. (MALARIA) Modeling Malaria Drugs using Genome-wide Transcriptional Response Profiles…..Page 25
56. (CHROMO) Chromosome Inversions and Adaptation……………………………………...…Page 26
57. (GENETIC) Developing High-density Genetic Maps in Non-model Systems……………………..Page 26

CSS – Computational Social Science

Projects with a Computational Psychology Focus…………………………………….….Page 27

58. Model fitting, model comparisons, and model selection uncertainty……………………………….Page 27
59. Bayesian Analysis of Large-scale Complex Educational Data……………………………………..Page 27

60. Data Mining Large-scale Educational Assessment Data……………………………………..……..Page 28
61. Intelligent Tutoring……………………………………………………………………………Page 28

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62. Interdisciplinary Center for Network Science & Applications…………………………..………Page 28
63. Racial, Economic, and Institutional Disparities in Home Mortgage……………………………..Page 29

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64. Large Overlapping Generations Models of Household Saving…………………………………..Page 29
65. General Equilibrium Structural Models and their Potential to Evaluate the Effects of Government Policy……………………………………………………………………………………Page 29

Projects with a Cyber Infrastructure (CI) for Social Sciences Focus…………………...…...Page 30

66. Digital Historical Architectural Research and Materials Analysis (DHARMA)……………..……..Page 30
67. Social Computing and Modeling & Simulation of Complex Social Systems…………………..…..Page 30
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69. Global Open Simulator…………………………………………………………………………..Page 70
70. Multicriteria Decision Making in Social Problems…………………………………..…………..…Page 70

PROJECT DESCRIPTIONS

Projects Offered for BOTH time frames

(8 week June 4th – July 29th AND 6 weeks July 2nd – August 12th)

College of Science

Department of Chemistry and Biochemistry

1. Discovering and Characterizing Protein Sequences that Stall the Ribosome

Description:
Every protein in the cell is synthesized by a ribosome. The newly synthesized protein first passes through the ribosome exit tunnel, a ~100 Angstrom tunnel that shields approximately 30 aa residues. For decades it was thought that this must be a "Teflon tunnel", in order to enable proteins of any sequence to pass through it without sticking. More recently, several specific protein sequences have been shown to stick to the wall of the exit tunnel and stall translation elongation, providing a novel mechanism to regulate protein production in vivo. This lab has developed a high-throughput screening strategy to identify novel translation stall sequences. The iSURE student working on this project will work alongside the professor and her graduate students to use this screen to identify

novel stalling sequences and determine their stalling mechanism, using approaches drawn from biochemistry, biophysics, molecular biology and microbiology.

2. Late-Transition Metal Pincer-Type Complexes Involving Metal-Ligand Cooperation for Alkane and Small Molecule Activation

Description:
Catalysis is at the center of green chemistry efforts, especially when it involves readily available feedstock such as water, alcohols, and amines. An approach with major practical implications is the selective functionalization of E-H (E = O, N, C, Si, B) bonds since syntheses can be simplified and less waste generated than with traditional methods. Oxidative addition of such bonds will be investigated. Our new approach involves metal-ligand cooperation, specifically, hydrogen transfer from the ligand to the metal and vice versa, which allows transformations under mild conditions.

3. Perovskite photovoltaics

Description:
In recent years, nanomaterials have emerged as the new building blocks to construct light energy harvesting assemblies. Efforts are being made to design high efficiency organic metal halide hybrid structures that exhibit improved selectivity and efficiency towards light energy conversion. This project will evaluate the performance of solid state cesium lead halide perovskite solar cells. The summer research involves synthesis of semiconductor nanocrystals and dissolution processed thin perovskite films on various oxide films and constructing solar cells. These cells will then be evaluated to establish their photovoltaic properties. The overall goal is to tune the photoresponse of the thin film solar cell through mixed halide composition and improve the solar conversion efficiencies. The student will be involved in the preparation of perovskite films, spectroscopic and material characterization, solar cell fabrication and performance evaluation. Applicants with chemistry/physics background at sophomore level are preferred.

4. Nanostructure assemblies for sensing application

Description:
Recent advances in the construction and characterization of graphene-semiconductor/metal nanoparticle composites in our laboratory has allowed us to develop multi-functional materials for energy conversion and storage. These next-generation composite systems may possess the capability to integrate conversion and storage of solar energy, detection and selective destruction of trace environmental contaminants, or achieve single-substrate, multi-step heterogeneous catalysis. This research project will involve synthesis of graphene based assemblies for photocatalytic and photovoltaic conversion of light energy. The graphene oxide-semiconductor assemblies will be characterized by transmission electron microscopy, and the excited state processes will be evaluated using time-resolved emission and absorption techniques. The goal is to optimize the performance of graphene based assembly and maximize the photoconversion efficiency. The student will be involved in the preparation of graphene-based semiconductor nanoassembly, spectroscopic and material characterization, and test the assemblies in sensing applications. Applicants with chemistry/physics background at sophomore level are preferred.

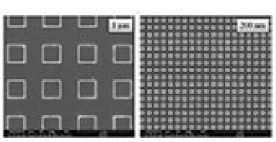
5. Identifying nanostructure in medieval manuscripts

Description:
The use of different molecular species has been used to provide color in illuminated works of art since ancient times. Distinct mineral particles, as well as organic dyes mixed with minerals are combined to provide color and decorate books and other manuscripts. The identity and composition of pigments may be linked to guilds and specific artisans. Interestingly, chemical differences associated with structure appear to play a key role in the observed properties. Using modern chemical characterization techniques, this project seeks to understand the correlation between molecular species and craftsmanship used to produce illuminated manuscripts dating from the middle ages. Interested students will be trained and use a variety of non-destructive spectroscopic techniques (e.g., Raman spectroscopy, hyperspectral darkfield imaging, and others) to examine and characterize the molecular properties in actual medieval manuscripts. This project is in collaboration with the Snite Museum of Art and the Notre Dame Nuclear Science Lab. This project is open to students at all levels, but familiarity with spectroscopy is helpful.

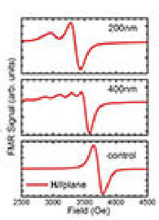
Department of Physics

6. Ferromagnetic semiconductor nanostructures

Description:
Our research program involves the investigation of ferromagnetic semiconductors, such as GaMnAs. Interest in these materials is motivated by the fact that they combine both the electronic properties of a semiconductor and the magnetism of a ferromagnet, and thus open the possibility of manipulating and storing information in a single monolithic structure. It is clear that as the dimensions of a ferromagnetic semiconductor device are reduced to nanometer scale, its magnetic properties will change dramatically. In the summer of 2017, we therefore plan to focus on a systematic investigation of this aspect of ferromagnetic semiconductors. In Fig. 1, we show an example of a thin ferromagnetic semiconductor film fabricated lithographically into nanometer scale elements. We plan to carry out basic structural, electrical and magnetic properties of structures of this type; and, in certain cases, also to carry out ferromagnetic resonance (FMR) measurements on selected specimens. Examples of FMR spectra obtained on specimens such as those shown in Fig. 1 are shown on the right of Fig. 1. Note the conspicuous change that has emerged in the spectra obtained as the sample was reduced. The additional peaks represent spin wave resonances, and provide basic information about magnetic surface pinning effects that occur as the size of our elements is reduced to nanometer scale. The student involved in our research will assist us in the design and fabrication, and in structural, magnetic and electrical measurements on ferromagnetic semiconductors we produce in our molecular beam epitaxy laboratory. Background in physics or electrical engineering will be sufficient for a meaningful involvement in this project.



Left: an example of lithographically-fabricated nanostructures of GaMnAs alloy.
Right: ferromagnetic resonance spectra observed on GaMnAs control film and on 200nm and 400 nm nanostructures.



7. Ecological control theory

Description:
Evolutionary control has a long history starting with agricultural domestication and culminating into contemporary genome editing technologies. However, this history is largely limited to controlling individual species. We view ecological and biosocial networks as the new circuit board, and evolution as a manufacturing process capable of fabricating eco-machines. Evolutionary control promises terraforming worlds, degrading pollution, and manufacturing astonishing compounds. This is a theoretical / computational project that aims to establish an analytical framework to steer the evolution of multiple populations that strongly interact with one other. Specifically, we wish to theoretically understand how to manipulate the connectivity of networks representing ecological or biosocial webs, which range from bacterial biofilms to rainforests. The project particularly focuses on ecological control under noisy or incomplete knowledge of the existing interactions and population levels of species. The project requires mathematical and computational dexterity. Applicants are expected to be familiar with matlab, differential equations / dynamic systems, and elementary probability theory.

College of Engineering

Department of Computer Science and Engineering

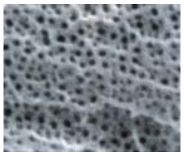
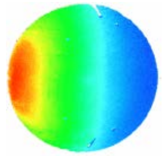
8. Visual Data Analytics

Description:
iSURE students familiar with programming in C/C++, OpenGL/GLSL/WebGL, or D3.js will assist in the design and implementation of visualization and analytics programs for analyzing and understanding a wide variety of data (e.g., simulation data, social media data), and for teaching and learning essential visualization concepts and techniques.

Department of Aerospace and Mechanical Engineering

9. Chemical sensor for fluid dynamic and environmental applications

Description:
This project is an interdisciplinary topic on chemistry and fluid dynamics. A chemical sensor gives luminescent output related to physical or chemical quantities, such as oxygen pressure, temperature, pH, oxygen, and carbon dioxide. It can be coated or sprayed onto a fluid dynamic or environmental object for testing. The sensor consists of a luminescent probe, porous material, polymer, and solvent. These components influence to the characteristic outputs of this sensor in terms of its signal level, signal sensitivity, and response time. It is desired to find the relationship among those components and characteristic outputs to create an optimum sensor for various testing.

The expected and/or anticipated involvement:
A student will be involved in a chemical sensor development and its characterization using spectrometer and pressure/temperature-controlled device. The developed senor will be tested in a shock tube.
Preferred discipline, expertise, lab skills:
A student from the following discipline is preferred: chemistry, chemical engineering, industrial engineering, mechanical engineering, aerospace engineering.

10. Molecular dynamics simulations of thermal transport at nanoscale

Description: N/A

11. Fabrication of polymer nanofibers with anomalous thermal conductivity

Description:
Amorphous polymers are known as thermal insulators with a thermal conductivity of ~0.1-0.3 W/mK. However, they can be more thermally conductive than many metals if we can reform them into highly aligned nanofibers (thermal conductivity > 50 W/mK). This suggests that polymers can be used to replace metals in many heat transfer devices and equipment, such as in electronic packaging and heat exchangers, with the additional advantages of reduced weight, chemical resistance, and lower cost. In this project, undergraduate researchers will fabricate polymer fibers with nanometer diameters by ultra-drawing fibers from polymer melt. They will also characterize the nanofibers using electron microscopes and X-ray scattering, and measure thermal transport properties using scanning thermal microscopy.

12. High throughput spray coating of membranes for applications in desalination and waste chemical recovery

Description:
Technical Objectives: Optimize and characterize a new spray coating system developed in the SST Research Lab for the high throughput processing of membranes. We have developed a piezoelectric-based spray system and developed a high throughput coating system for membranes. This research will focus on optimizing the process conditions (spray rate and duration, number of coatings, solution chemistry).
REU Role: Conduct spray experiments and membrane characterization and draw conclusions about optimal manufacturing process in collaboration with graduate student or post-doc.

Preferred discipline(s), expertise, lab skills, etc.: Any science and engineering discipline is acceptable, although those with a background in chemistry and/or electrical engineering are preferred. Student must be willing to work primarily on experiments in a very detailed and systematic manner.

13. Electrical characterization of plasma behavior in catalyst systems

Description:
Technical Objectives: Characterize plasma behavior in catalyst systems using various electrical measurements. Catalyst systems such as those used for the production of synthetic gas from methane and carbon dioxide or ammonia from nitrogen and hydrogen can be enhanced by a plasma (gas discharge). This research will focus on understanding this enhancement at a fundamental level by correlating electrical behavior in the plasma to catalysis enhancement.
REU Role: Conduct plasma experiments under different conditions and take electrical measurements of the plasma behavior in collaboration with a graduate student or post-doc.
Preferred discipline(s), expertise, lab skills, etc.: Any science and engineering discipline is acceptable, although those with a background in electrical or chemical engineering are preferred. Student must be willing to work primarily on experiments in a very detailed and systematic manner.

14. Optical characterization of plasma behavior in catalyst systems

Description:
Technical Objectives: Characterize plasma behavior in catalyst systems using an optical technique called optical emission spectroscopy. Catalyst systems such as those used for the production of synthetic gas from methane and carbon dioxide or ammonia from nitrogen and hydrogen can be enhanced by a plasma (gas discharge). This research will focus on understanding this enhancement at a fundamental level by correlating the light produced by the plasma to catalysis enhancement.
REU Role: Conduct plasma experiments under different conditions and take optical measurements of the plasma behavior in collaboration with a graduate student or post-doc.
Preferred discipline(s), expertise, lab skills, etc.: Any science and engineering discipline is acceptable, although those with a background in electrical or chemical engineering are preferred. Student must be willing to work primarily on experiments in a very detailed and systematic manner.

15. Custom-built reaction chambers and in situ monitoring tools

Description:
The reactions carried out in a liquid media have, thus far, been performed in either a three neck flask or a beaker. The goal, however, is to veer away from the use of standard glassware and, instead, carry out syntheses in enclosed reaction chambers that offer a more controlled reaction environment, versatility and in situ diagnostics. The final system will be able to: (i) flow a series of reactants into and out of a reaction chamber using syringe pumps without ever exposing the structures to air, (ii) heat an anchored substrate as well as the surrounding liquids, and (iii) perform a sparging procedure prior to reactions involving easily oxidized metals. The system will use a

Teflon-based reaction vessel instead of glassware because Teflon provides both chemical compatibility with the reactions being performed and machinability. The latter property is crucial in that it allows for the use of O-ring seals, threaded connectors and internal components with more complex geometries (e.g., a substrate holder). Preferred disciplines(s): mechanical engineering, chemistry, chemical engineering, materials science and machining.

16. Nanoparticle contrast agents for quantitative molecular imaging with CT

Description:
Molecular imaging with computed tomography (CT) could offer a single, low-cost and widely available modality for combined molecular and anatomic imaging at high spatiotemporal resolution. Nanoparticles (NPs) comprising high-Z metals, such as Au, have gained recent interest as X-ray contrast agents due to enabling the delivery of a greater mass payload compared with molecular contrast agents used clinically. Concomitant developments in photon-counting spectral CT are also transforming the capabilities of CT by providing quantitative multi-material decomposition. Therefore, students on this project will investigate the design, synthesis, and application of NP contrast agents for quantitative molecular imaging with CT. Core-shell NPs are designed for strong X-ray contrast, biostability, multimodal/multi-agent imaging, and targeted delivery. Applications include quantitative molecular imaging of multiple probe/tissue compositions, specific cancer cell populations (e.g., HER2+ breast cancer cells, cancer stem cells, etc.), tumors, associated pathologies (e.g., microcalcifications), drug delivery, and biomaterial degradation using both conventional CT and photon-counting spectral CT. Students will also interact with collaborators at the IU School of Medicine in South Bend and/or the Loyola University Medical Center in Chicago.

Department of Aerospace and Mechanical Engineering / Department of Electrical Engineering

17. Phononic nanoparticles for low-loss, tunable nanophotonics in the mid- and far-IR

Description:
Phononic nanoparticles are a new class of optical materials with untapped potential for realizing new mid- and far-infrared detection and sensing nanotechnologies that are functionally analogous to ultraviolet and near-infrared plasmonic nanotechnologies but with even greater sensitivity. Phononic nanotechnologies have potential applications in analytical chemistry, biomedicine, environmental science, homeland security, astrophysics, and geology. However, basic scientific knowledge of the governing structure-property relationships for engineering the optical properties of phononic nanoparticles are not well understood or developed. Therefore, students on this project will investigate the optical properties of candidate phononic materials using both modeling and experimental characterization of synthesized nanoparticles. As such, this interdisciplinary research experience will cut across both materials science and optical science.

Department of Electrical Engineering

18. RadioHound: A low-cost sensor network for mapping the radio spectrum

Description:
RadioHound is a project involving several faculty and students at the University of Notre Dame, where a network of sensors is being designed and built for mapping radio spectrum usage in the most-used frequencies. The ultimate goal is to create a map of spectrum usage across large geographic areas and for long periods of time. The project involves the design of hardware and software for control, visualization, and storage of large amounts of captured spectrum data.

19. Design and analysis of high-performance compound semiconductor devices

Description:
Numerical simulation and optimization of high-performance III-V compound semiconductor devices will be performed. Specific devices include photovoltaics, high-speed transistors, high voltage diodes and transistors, and novel devices for low-power digital and signal processing.

20. Fabrication process development for high-performance devices

Description:
Student will contribute to development of fabrication processes for high-performance III-V compound semiconductor devices, working in Notre Dame's cleanroom facility. Specific devices include high voltage diodes and transistors, as well as RF/microwave devices.

21. Micro-fabricated negative-index metamaterial lenses for passive near-horizon beam-steering

Description:
As the demand for mobile data continues to grow at exponential rates the wireless industry is looking toward the millimeter-wave regime (50-90 GHz) to access untapped spectrum (up to 20 GHz of contiguous spectrum) to meet this demand. One of the key challenges of millimeter-wave systems is the increased path loss (20log (f)) at high frequencies compared with current sub-6 GHz wireless networks. A proposed solution is to employ highgain antenna arrays that compensate for the path loss but have a corresponding narrow beam width. To maintain a wireless link with a mobile device beam-steering is employed. Traditional beam-steering uses active phased arrays that incur high cost and power dissipation. An alternative to active phased array beam-steering antennas is the passive Luneberg lens which boasts zero power dissipation, low loss, and high gain. However, the Luneberg lens is a 3D (spherical) gradient index lens traditionally requiring elaborate machining of concentric shells of dielectric. Due to the difficulties of fabrication, this lens has traditionally only been realized in bands below 20 GHz. Recently, the method of transformation optics has been presented as a means of physically distorting an electromagnetic structure and maintaining its functionality by spatially varying the permittivity throughout the structure. This has enabled the design of flat lenses but they require so-called gradient index optics. Over the past year, we have developed a process for manufacturing gradient index optics targeting the millimeter-wave bands

from 30-150 GHz. The approach is known as perforated media, as shown in the figure above. With such a structure, we can vary the permittivity in a 2D plan (a wafer), and by stacking multiple wafers we can vary the permittivity throughout a 3D structure. So far, our approach is able to achieve only "ordinary media" ($\varepsilon r>=1.0$), which enforced certain limits on the maximum angle that a beam can be steered. To steer a beam to the horizon, permittivity must be allowed to exceed the ordinary limit. By integrating vertical metallization in the etched voids, we can incorporate the so-called "thin-wire" metamaterial unit-cell into our structure and achieve $\varepsilon r<1.0$ and even $\varepsilon r<0$. This provides additional flexibility to achieve near-horizon beam-steering. Working in NDnano's state-of-the-art nanofabrication facility, and in conjunction with one or multiple graduate students, the student will perform design simulations, mask design, pattern generation, lithography, etching, and measurement in support of three technical objectives for this project:

1. In conjunction with the faculty advisor and graduate student mentor, develop the theory for the design of the negative permittivty unit cell

2. Simulate the design in a full-wave electromagnetic solver (e.g., Ansys HFSS)

3. Fabricate and measure the new negative (or reduced) permittivity unit cell in the cleanroom

Not only will the work in this project complement ongoing research, but it will also provide an enabling technology for many follow-on projects. A rising junior or senior with electrical engineering background is expected but qualified candidates from all levels will be considered. Given the nature of microfabrication tasks, the undergraduate student will team with at least one graduate student to provide continuity and additional effort applied to the task.

22. Steep-slope ferroelectric transistors

Description:
The recent experimental detection of negative differential capacitance in ferroelectric dielectrics rekindles our hopes that the phenomenon can be harnessed to push transistor scaling and energy-efficient nanoelectronics. The unstable negative capacitance of the ferroelectric has been predicted before, but its direct measurement is elusive. However, one can stabilize the negative capacitance of ferroelectric by putting it in series with the positive channel capacitance of the transistor. Recently in our group, we have developed a novel ferroelectric dielectric that is integrated directly within the gate stack of a silicon transistor to form a ferroelectric field-effect transistor. In this proposed project, the researchers will have an opportunity to characterize the Ferro FETs in detail and participate in developing device physics based simulation models of the resulting Ferro FETs. The student should have taken an undergraduate course in semiconductor device physics or equivalent. Preference will be given to students who have some experience in electrical characterization of transistors, diodes, capacitors, inductors, etc.

23. Noise measurements in nanoscale single-electron devices

Description:
Single electron tunneling transistors (SET) are quantum mechanical devices that are capable of detecting a tiny displacement of charge (much less than one electron!) in a nearby nanostructure coupled to it. But this unique capability of an SET sensing device is limited by noise. Noise is a fascinating phenomenon where the physical

system exhibits random fluctuation of its parameters, which in the case of sensors like SET, ultimately limits its ability to act as a detector. By carefully designing parameters of the SETs, one can improve their immunity by orders of magnitude. But what are the underlying physical mechanisms that lead to a drastic difference in performance, like shown in the figure (right)? Projects this group study the connections between SET fabrication steps and resulting device performance, and explore the limits imposed by various sources of noise on the performance of the SET devices. The projects will include building circuits (amplifiers and filters) for noise measurements at different temperatures (from room temperature, 300K down to a very low, 0.3K) as well as the actual measurements of SETs and data analysis. A student involved in these projects will gain experience in hardware design and implementations, device measurement and data analysis techniques, and some programming. Students will work on the experimental measurements, data analysis, construction of circuits, and writing control programs. Students with backgrounds in physics, electrical engineering, and computer science are preferred. Some knowledge of programming, data analysis and soldering is helpful.

24. Automated testing of tunnel field-effect transistors

Description:
The student will work with graduate students and post docs to advance the development of tunnel field-effect transistors (TFETs). These transistors are more energy efficient than the Si MOSFET. The student will use a Cascade autoprober, which allows step and repeat probing of devices on chip, and learn an integrated measurement software called Wavevue for control and analysis of the data. The goal of the project is to develop automated measurement routines and methods to extract key performance measures for the transistors, and then generate automated reports that students can use to document progress. The student will learn transistor testing, measurement automation, and data analysis to understand the physics of TFETs. Preferred discipline(s), expertise, lab skills, etc. Applicants with the ability to learn software, an interest in semiconductor devices and automated current-voltage and capacitance-voltage testing, and the ability to solve problems are preferred.

25. Energy recovery for ultra-low energy computation

Description:
Anyone who owns a laptop knows that power dissipation and the associated heat are a problem for the microelectronics industry. As electronic devices scale down in size, they use less power (and hence energy), but is there a lower limit to the energy that must be dissipated by each device? Recent experimental measurements have demonstrated our ability to measure energy dissipation in the range of a ~15 yJ (1 yJ is 10-24 J), and we are building CMOS circuits to operate in this range. Projects in this group will explore the limits of ultra-low power computing, and designing, building and measuring circuits that test these limits, and clock circuits that can recycle the energy used in computation. The projects will include building circuits and amplifiers for energy measurements of the CMOS circuits as well as the actual measurements. The project will also include the design of the next generation of the adiabatic circuits. A student involved in these projects will gain experience in programming, CMOS design, and device measurement techniques. Students will work on the construction of circuits, writing control programs, and making measurements. Students in electrical engineering, physics, and computer science students are preferred. Some knowledge of programming and soldering is helpful.

Department of Chemical and Biomolecular Engineering

26. Polymer electrolytes for advanced rechargeable batteries

Description:
The objective of the research is to investigate solid polymer electrolytes for use in lithium and/or magnesium rechargeable batteries. Such electrolytes have to potential for increase battery safety due to their lower volatility and higher thermal stability compared with commercial electrolytes. Current polymer electrolytes suffer from low ionic conductivities that result in low battery charge/discharge rates, which preclude their use in commercial devices. This project will investigate ion transport mechanisms in novel single-ion conducting polymer electrolytes. The REU student will prepare materials and characterize the electrochemical and thermal properties in these new materials. Prior lab experience and a background in chemical engineering, chemistry, materials science, or a closely related field is preferred.

27. Dendrite growth in rechargeable lithium metal batteries

Description:
Widespread commercialization of high energy density rechargeable lithium metal batteries has been prevented for decades due to lithium dendrite growth. Lithium metal electrodeposits unevenly in many conditions, leading to growth of lithium dendrites that can short-circuit the battery and result in fire or explosion. The parameters affecting lithium dendrite growth are still not well understood. This project will investigate the effects of polymer electrolyte characteristics on dendrite nucleation timescales. The REU student will prepare polymer electrolyte films, fabricate lithium metal batteries, and conduct short-circuit testing. Prior lab experience and a background in chemical engineering, chemistry, materials science, or a closely related field is preferred.

28. Effects of Acidity and Salinity on Polymer Drug-Delivery Complexes

Description:
A host of interesting phenomena, both biological and technological, involve the complexation of charged polymers; these may be long polymers with well-defined secondary structure, such as proteins, linear polyelectrolytes, or multi-branched species. A particularly interesting phenomenon within polyelectrolyte solutions is coacervation, a liquid–liquid phase separation where polymer-enriched liquid droplets are formed within a dilute phase. Coacervation is a puzzling process where two primarily aqueous phases become immiscible. Aggregates (coacervates) formed in mixtures of oppositely charged polyelectrolytes are known as complex coacervates. Coacervates occur in many natural systems and have found application in microencapsulation and extraction processes, as their ultra-low surface tension allows them to readily assimilate nanoparticles or drug payloads within aqueous suspension. Coacervation is intimately related to the process of layer-by-layer deposition, where films up to micrometers in thickness are built by iterative surface adsorption of polyelectrolytes. Such films are of interest as solid electrolytes in lightweight batteries fuel-cell electrodes protective coatings and drug micro-encapsulation.

This topic inspires REU projects involving characterization of coacervates through molecular dynamics simulation. These are focused on the use of complex coacervates in the delivery of therapeutic compounds to specific biological targets, as the highly charged, condensed environments they facilitate can act to stabilize and protect molecular and macromolecular species.

1. Using a customized version of the LAMMPS open-source molecular simulation package, LAMMPS25 the student will examine the role of pH in the complexation of long polyions in the presence of added salt. Of particular note are the connections between molecular structure and effective pKa in dilute and concentrated solutions, as this quantity determines the useful phase window for coacervates as a host material for drug delivery applications.
2. A second project involves the influence of the highly charged environment provided by a complex coacervate in stabilizing drugs—in particular protein based therapies—against deactivation and degradation. The student will explicitly determine how these environments affect the pKa and native structure of therapeutic compounds using coarse-grained and fully atomistic models.

It is preferable (but not required) for students interested in this project to have prior experience with writing computer code (C++ preferred) and with scripting languages such as python and bash to facilitate running computations on the Whitmer group cluster and CRC machines.

29. Performance of Functional Metal–Organic Frameworks

Description:
The beautiful and intricate geometries of metal–organic frameworks (MOFs), together with their impressive capacities for energy storage, carbon sequestration, and catalysis, inspire their study in equal amounts. This array of applications is facilitated by the open structure of the MOF and the myriad choices of linking molecules. In this project, we will examine the properties of some recently synthesized open structures, including the ZnO2/pyridine carboxylate structures. Of particular interest are the adsorption free energies and diffusion constants for compounds within these lattices, as they will influence operating conditions and capabilities of the MOF structure. During the REU, the student will build molecular simulation models and learn techniques for statistically characterizing the properties of crystal lattices, in addition to thermodynamic integration and manifold reduction methods. The student will be expected to have some familiarity with writing computer codes, preferably in C++. Beyond this, only general knowledge of physics and chemistry is required.

30. Predicting Material Elastic Responses from Molecular Simulations

Description:
Elastic materials exhibit a restoring force which opposes applied stress, resulting from a perturbation away from thermodynamic equilibrium. Materials may exhibit different types of elasticity depending on their character. Each opposed deformation defines an elastic modulus; liquid crystals may have three or more elastic moduli characterizing their response to curvature deformations in their ordering field; solids, both crystalline and amorphous, also have several elastic moduli, such as the bulk modulus, shear modulus and Young's modulus. Each of these moduli may be related to derivatives of the system's free energy relative to a variable characterizing the extent of deformation. The group has three potential projects related to measurements of elastic properties in silico, which build on recent formalisms utilizing free energy perturbation simulations to extract the elastic

coefficients of liquid crystals into the domain of two dimensional membranes and three dimensional solids. We aim to characterize the typical elastic properties of each phase, and validate our data against previous simulations and theoretical models.

In particular, the three projects are:

- Application of free-energy perturbations to atomistic models of liquid crystals to predict elastic constants in silico, and contribute to development of a high throughput workflow for elastic property screening.
- The utilization of recently developed coarse-grained models of biological membranes to understand the enthalpic interactions and entropic packing alter the elastic behavior of a membrane. This project also seeks to demonstrate the effectiveness of "flat-histogram" methods6 relative to fluctuation methods in determining surface tension and elasticity of membranes.
- Ionic liquid crystals, salt species which self-assemble into phases with charged and uncharged domains, have recently been of interest as novel battery electrolytes. Here we will examine the response behavior of self-assembled phases in the ionic liquid crystal [C16mim] [PF6], to obtain structure–property relationships which will be useful in processing these materials.

During the summer REU, the student will work intensively on molecular simulation models and learn techniques of advanced sampling, in particular flat-histogram methods used for the measurement of free energies. The student will be expected to have some familiarity with writing computer codes, preferably in C++. Beyond this, only general knowledge of physics and chemistry is required.

31. Engineering multifunctional nanoparticles for targeted drug delivery in cancer

Description:

Modern cancer therapeutics are typically developed to aim at key pathways and proteins that are critical to the survival and progression of malignant cells. Nevertheless, they are still associated with undesirable side effects due to non-specific toxicity that non-targeted tissue and organs experience. In recent years, nanoparticle (NP) based drug delivery systems that carry drugs to tumors in the body have greatly improved the efficacy of traditional therapeutics while decreasing the associated systemic toxicities. NPs with a diameter of 10-200 nm can selectively target and preferentially home at the tumor site via the enhanced permeability and retention (EPR) effect. More complex NPs, such as multiple drug carriers (for combination therapy) and coatings of targeting elements for receptors on cancer cells, have also been engineered to improve the overall outcome by overcoming problems associated with tumor tissue targeting and penetration, drug resistance, cellular uptake and circulation half-life. We use NPs to target multiple myeloma (MM), a B-cell malignancy characterized by proliferation of monoclonal plasma cells in the bone marrow (BM) and is the second most common type of blood cancer in the U.S. Despite the recent advances in treatment strategies and the emergence of novel therapies, it still remains incurable. A major factor that contributes to development of drug resistance in MM is the interaction of MM cancer cells with the BM microenvironment. It has been demonstrated that the adhesion of MM cells to the BM stroma via $\alpha 4\beta 1$ integrins leads to cell adhesion mediated drug resistance (CAM-DR), which enables MM cells to gain resistance to drugs such as doxorubicin (Dox)–a 1st line chemotherapeutic in the treatment of MM. To overcome this problem, the clinicians apply combination therapy, which is the simultaneous use of two complementary chemotherapeutic agents during treatment. One caveat of this treatment method has been that it is almost impossible to attain the critical stoichiometry at the tumor that is necessary to achieve this synergistic drug effect when conventional methods of chemotherapy are used. Here, we seek to overcome this challenge by using an engineering approach for targeted drug delivery. The overall objective of this proposed project is to engineer "smart" nanoparticles that will deliver and exert the cytotoxic effects of the chemotherapeutic agents on MM cells, and at the same time do it in such a manner as to overcome CAM-DR for improved patient outcome. To enable this, we will engineer micellar nanoparticles that will be (i) functionalized with α4β1-antagonist peptides as well as Dox and carfilzomib drug conjugates, and (ii) designed to show the adhesion inhibitory and the cytotoxic effects in a temporal sequence. When the nanoparticles are delivered to the MM cells, as a first step they will interact with the cell surface α4β1 integrins and inhibit MM cell adhesion to the stroma, thereby preventing development of CAM-DR (Fig. 1). In the second step, the chemotherapeutic agents will exert their synergistic cytotoxic effects after cellular uptake, as the nanoparticles will be designed to require a low pH environment such as the endocytic vesicles, to release active drugs. This way, the "smart" nanoparticles will act on the MM cells in a temporal fashion and prevent development of CAM-DR for improved patient outcome.

32. Microporous membrane reactors for antibody digestion and characterization

Description:
Antibodies are the fastest growing class of therapeutic drugs. Due to the complex composition and biosynthesis of these drugs, quality control is vital to ensure that antibodies are effective and do not induce side effects such as an immune response. Mass spectrometry is the most powerful tool for antibody characterization, but it usually requires antibody digestion into smaller pieces that are amenable to characterization. This research aims to use membrane reactors to control antibody proteolysis and create a few large peptides that enable rapid detection of antibody modifications such as oxidation, phosphorylation, and glycosylation. Controlled digestion may also identify changes in protein conformation or the formation of disulfide bonds. The project will likely include immobilization of enzymes in membranes, performing digestion reactions and mass spectrometry, and interpreting mass spectrometry data. The research is particularly appropriate for students in chemical engineering, chemistry, or biochemistry.

33. Nanostructured polysulfone polyelectrolyte copolymer membranes for fuel cells

Description:
Sulfonated polysulfone copolymers with controlled nanophase-separated morphology hold great potential as alternatives to benchmark Nafion® for polyelectrolyte membrane fuel cells (PEMFCs) due to their much better proton conductivity at low relative humidity (RH) levels and thermal stability. Previous research has shown that long hydrophilic (ionic) sequences or a high degree of sulfonation are needed to form well-connected proton conducting nanochannels that enable high proton conductivity at low RH. However, it invariably comes at the expense of high water uptake and excessive membrane swelling, resulting in deterioration of the dimensional stability and mechanical robustness. This project aims to exploit an innovative supramolecular strategy to address this water management challenge in PEM membranes via introducing triptycene-based building blocks into polymer backbones. It is expected that supramolecular interactions of chain threading and interlocking induced by triptycene units can effectively suppress water swelling while maintaining high water uptake, which is critical to provide high proton conductivity under low RH conditions. Specifically, both random and multiblock

copolymers of systematically varied compositions will be developed in this project to investigate how supramolecular interactions of triptycene units govern the formation of proton-conducting nanochannels as well as proton transport properties. The project will start with the synthesis of triptycene diol monomer, which will be copolymerized with commercial sulfonated monomer to produce both random and multiblock copolymers. Comprehensive characterizations of the copolymers will be conducted to confirm the chemical structure (NMR ad FTIR) and access their thermal and mechanical properties (DSC, TGA, tensile test, etc.). Membrane fabrication and acidification will then follow to prepare free standing, defect-free films for water swelling measurement, morphology characterization (AFM, TEM) and proton conductivity measurements (impedance spectroscopy). A student in materials science, chemical engineering, or chemistry is preferred, and having previous experience in a chemical laboratory would be helpful.

34. Polymer membranes with tunable microporosity for gas separations

Description:
Polymers with well-defined microporosity are highly desired for gas separation membranes, wherein high microporosity enables fast gas transport while the finely tuned pore size regulates selective transport via size sieving. Recently there have been markedly increasing research interests in developing microporous polymers for gas separation membranes, such as polymers with intrinsic microporosity (PIMs). However, the reportedly super high gas permeability of microporous polymers is always accompanied by low selectivity, mainly due to the lack of precise control over pore size distribution in these polymers. Moreover, physical aging induced deterioration of permeability remains as one of the biggest challenges for microporous polymer membranes. This project will focus on constructing highly rigid ladder-like polymers using a shape-persistent building block based on pentiptycene-containing structural units. The novelty of this new type of microporous polymers lies in the truly intrinsic microporosity defined configurationally by the shape of the pentiptycene units, which offers unique opportunity to tailor the microcavity architecture in the membranes and simultaneously provide superior resistance towards physical aging by taking advantage of the rigid framework of pentiptycene moieties. The project will involve the synthesis of pentiptycene-based monomers with various bridgehead substituent groups, polymerization of tetrafunctional pentiptycene monomers with commercial comonomers, membrane fabrication/characterization, and pure-gas permeation tests. A student in materials science, chemical engineering, or chemistry is preferred, and having previous experience in a chemical laboratory would be helpful.

35. Fabrication of solid-state batteries

Description:
Solid state batteries (SSBs) may be a key enabler for electric vehicles. A solid electrolyte can overcome many shortcomings of present technology including offering wider electrochemical voltage ranges, better chemical compatibility, and improved safety. Progress is needed to overcome electrolyte limitations and provide more economical processing while still delivering sufficient energy density for automotive application. ND researchers are developing ceramic materials (Li7La3Zr2O12) and low-cost processing methods to provide for high-power, solid-state, lithium-ion batteries for use in EVs. A key factor to drive down costs is the development of scalable, ceramic fabrication techniques. The goal of this project is the chemical processing and sintering of nanosized electrolyte and electrode powders for development of composite electrode microstructures to yield high-

performance batteries. Liquid phase sintering of electrolytes has been developed to reduce required processing temperatures. Composite electrodes will be developed to permit co-sintering of electrode-electrolyte structures. The student will synthesize (chemical processing) and characterize (X-ray diffraction, dilatometry) nano-sized powder of battery component materials (electrolytes, eletrodes). Slurries for tape casting will be prepared and sintered. Cast tapes will be characterized (impedance spectroscopy). Batteries will be fabricated from tapes (glove box work). Preferred disciplines: materials science, chemical engineering, chemistry.

36. Elucidating fundamental transport properties of copolymer-derived charge mosaic membranes

Description:
Nanoporous membranes based on self-assembled copolymer precursors are an emerging class of promising separation and purification devices, which will find application in water purification, pharmaceutical, and biofuel processing applications, due to the ability of researchers to control the nanostructure and chemistry of these multifunctional materials. To date, the most successful methodology for directing the assembly of nanostructured copolymer-based membranes has been the self-assembly and nonsolvent induced phase separation (SNIPS) procedure. This membrane fabrication protocol combines the thermodynamically driven self-assembly of copolymers in solution with the oft-used nonsolvent induced phase separation membrane fabrication technique. In addition to being facile and scalable, the versatility of the SNIPS process makes it an attractive membrane fabrication methodology. In particular, the membrane nanostructure and chemistry generated by the SNIPS process can be tuned by varying a number of engineering parameters. Recently, it was demonstrated that this flexibility could be exploited to generate charge-mosaic membranes based on the copolymer material platform. Charge mosaics contain both positively-charged and negatively-charged domains that traverse the thickness of the membrane. This structure enables both the cation and anion from a dissolved salt to permeate through the membrane without violating the macroscopic constraint of electroneutrality, and results in membranes that permeate dissolved salts more rapidly than solvent or neutral molecules. Unfortunately, the fundamental knowledge regarding how these membranes function is lagging. As such, the objective of this project is to identify the key material relationships that control the interplay between membrane nanostructure, functionality, and transport properties for charge mosaics membranes. The student researcher will be asked to fabricate membranes using the SNIPS process, and elucidate how the nanoscale structure and chemistry of the membranes impact the observed transport properties through experimental water flow and solute throughput tests. Chemical, mechanical, and environmental engineers are well-suited to undertake this research project.

37. Targeting therapeutic nanoparticles through supramolecular affinity

Description:
We are motivated to advance the practice of therapeutic nanotechnology by capturing several of the benefits of antibody targeting while avoiding some known complications. Antibodies are used for targeting due to high affinity and biological tissue-specificity. There are, however, downsides to antibody use in nanomedicine that could present issues in application moving forward: (i) Antibodies are fundamentally opsonins, a bio-recognizable signal that promotes cell-mediated uptake and clearance of foreign particles (e.g., viruses) by the reticuloendothelial system. Can we use alternative high-affinity targeting groups that would not be subjected to active biological clearance? (ii) A typical therapeutic nanoparticle (diameter ~50-100 nm) endowed with

antibodies (hydrodynamic diameter of ~10 nm) would be expected to have its surface properties and function altered by addition of this bulky appendage; furthermore, there is limited area on the nanoparticle surface to attach such a large targeting group. Can we design targeting based on minimal groups that have comparable affinity while limiting impact on the properties of the functional nanoparticle? Using ultra-high affinity supramolecular interactions as a type of "molecular Velcro," our group envisions a new therapeutic nanoparticle targeting axis built on minimal small molecule affinity motifs that serve as drivers of localization, in lieu of large targeting antibodies, while at the same time not sacrificing any affinity relative to an antibody-antigen interaction. An undergraduate working on this project will be expected to learn techniques for formulating synthetic nanoparticles to contain drugs and quantifying drug release using a combination of spectroscopy and chromatography. Additionally, this individual will be tasked with validating this mechanism for targeting in vitro through microscopy of fluorescent nanoparticles on cultured cells. Disciplines related to chemistry, chemical engineering, materials science, or bioengineering are encouraged to apply. A minimum of some prior laboratory coursework is expected.

38. Engineering responsive peptide-based drug nanocarriers

Description:
We are motivated to improve therapeutic specificity of self-assembling drug nanocarriers by endowing them with units that can promote a change in assembly state as a function of the presence of disease-relevant analytes and biomarkers. Typical nanocarriers for drug delivery demonstrate equilibrium-driven release. This is inefficient at best, and at worst can result in the accumulation of drug off-target in the body where it can elicit side-effects. Can we use disease-specific indicators to facilitate increased drug release specifically at the site of disease, toward non-equilibrium, responsive drug delivery? Peptide self-assembly affords one means to create nanostructures, and by virtue of these being based on non-covalent interactions, the energy barrier that must be overcome to induce a change in assembly state is modest relative to a system constructed covalently. Furthermore, peptide nanostructures can be designed with control over shape, interfacial curvature, and aspect-ratio. Our objective in this project is thus to incorporate analyte-sensing chemical units within a peptide backbone such that presence of the specific analyte drives a change from an assembled peptide-based drug carrier to a disassembled monomeric form accompanied by burst release of a drug. An undergraduate working on this project will be expected to learn techniques in solid-phase peptide synthesis, conduct routine characterization to study changes in material properties as a function of analyte concentration, and quantify the loading and release of drugs from these nanostructures using a combination of spectroscopy and chromatography. Disciplines related to chemistry, chemical engineering, materials science, or bioengineering are encouraged to apply. A minimum of some prior laboratory coursework is expected.

College of Arts and Letters

Department of Psychology

39. Cognitive Neuroscience of Memory & Aging Lab

Description:
Our lab uses behavioral testing, neuroimaging (EEG/ERP, fMRI), and neurostimulation (TMS, tDCS) techniques,

as well as statistical modeling (MVPA, CFA, SEM), to develop and test theories of memory. Our research is generally focused on memory and age-related changes in memory. In particular, we study the behavioral and neural processes associated with working memory and the relations among working memory, episodic memory, prospective memory, and higher-order cognition (e.g., fluid intelligence, language comprehension). We study these topics in various populations including young adults, healthy older adults, and in patients with Alzheimer's disease, Parkinson's disease, or amnesia. In your application, please comment on proficiency with computer programming. Experience with Matlab and/or Python is highly desired. Responsibilities will include helping lab members prepare applications, program experiments, run experiments / collect data, process data, and attending lab meetings.

40. Online Statistical Power Analysis for Simple and Complex Models

Description:
This project develops online software for power analysis with applications in psychology, education and health research (http://webpower.psychstat.org). Students should possess basic knowledge in programming, e.g., having taken a course in C/C++/C#, Java, Python, etc. Additional information about the lab can be found at http://nd.psychstat.org/research/index

Projects Offered for 8 week timeframe

Center for Research Computing (CRC) REU Program Projects

(8 week June 4th – July 29th)

Note: Only students who will be able to attend the program from June 4th – July 29th can apply to the following projects:

DISC – Data Intensive Scientific Computing

Projects with a Computer Science Focus

41. (VIS) Data Visualization

Description:
If "a picture is worth a thousand words", why not make data analytics visual for users so that they can easily explore data and assimilate information? In this project, students will gain valuable experience and practical skills in creating visual display of big data sets. Project topics include: (1) ND-GAIN Visualization: Using D3.js, this interactive tool will enable analytical reasoning of different countries' adaption to climate-related changes through customized visualization and comparison of the ND-GAIN index data; and (2) Eye-tracking Data Visualization: This project will transform eye-tracking data collected among the participants into graphs for matching and comparison with the goal of identifying common patterns and abnormal behaviors (e.g., mind wandering). (3) Graph Visualization for Education, using WebGL to teach graph visualization concepts through interactive

modules and auto-grading functions; These projects require programming skills in C/C++ or Java and preferably a graphics programming language such as OpenGL, WebGL, GLSL, or D3.js

42. (CYBER) Distributed Data and Cloud Based Cyber infrastructure for Science

Description:

This project's research addresses the growing economic, social and environmental costs to provision, power and operate cyber infrastructure in the United States; the utility costs alone are forecasted to exceed 7 billion dollars. The Environmentally Opportunistic Computing (EOC) approach integrates computing hardware with existing facilities and societies to create heat where it is needed, exploit available free cooling, utilize power wherever it is least expensive, and to provide computational capability for science at the optimal $/FLOP or $/TB ratio. These distributed infrastructures are inherently data locality and network capability sensitive. REU participants will have the opportunity to develop and advance data and network aware CI tool sets leveraging EOC to provide sustainable CI for computational science. The project requires familiarity with the Linux operating systems, and a willingness to tinker with virtual machines and system software to develop working systems.

43. (DISTSYS) Distributed Systems for Scientific Computing

Description:

The Cooperative Computing Lab designs open source software that enables high productivity computing on thousands of machines harnessed from clusters, clouds, and grids. Examples include the Makeflow workflow system, the Work Queue execution system, and the Parrot virtual filesystem. Learn how to use these tools run construct programs that run on hundreds to thousands of machines, then contribute to the design and development of this software used around the world for science and engineering. Some experience programming in C or Python is necessary. (Department will also offer training on these tools for use by students working on other REU projects.)

44. (BIOMETRICS) Data-Intensive Deep Learning for Biometrics

Description:

REU students will work with faculty and graduate students in the Computer Vision Research Laboratory (CVRL) to train and deploy deep neural network architectures for face detection/recognition/expression classification in the CVRL orpus of millions of face images and videos. Research will take advantage of local and/or cloud-based computing resources to investigate explicitly the issue of scaling. The desired outcome of this work is a corpus of developed software with good documentation and a clean draft of a research paper suitable for submission to a top-flight computer vision or biometrics conference such as CVPR, ICCV, or BTAS.

45. (NETSCI) Network Science for Computational Biology

Description:

Networks are everywhere! There exist social networks such as Facebook that link together Facebook users, technological networks such as the Internet that link together computers world-wide, and molecular networks that model interactions between genes and proteins in the cell. And networks are fun! For example, both graphite and diamond are composed of carbon atoms, but what gives them different properties (graphite being soft and dark, diamond being hard and clear) is the links between the atoms, i.e., the network. So, what do we do with networks? This group mines real-world networks and molecular networks in particular. Potential summer projects include: 1) developing novel computational strategies (or algorithms) for network comparison and alignment; 2) developing novel algorithms for dynamic network analysis, and 3) applied questions related to studying aging and disease. Mathematical and programming skills are required, prior biological experience is not needed.

Projects with a Physics Focus

46. (LOBSTER) Crunching LHC Data on 25K Cores with Lobster

Description:
The need for computing resources at the Large Hadron Collider (LHC) is rapidly outpacing the available funding. The Large-scale Opportunistic Batch Submission Toolkit for Exploiting Resources (Lobster) software has enabled physicists analyzing data from the Compact Muon Solenoid (CMS) experiment at the LHC to leverage the roughly 25,000 CPU cores available as opportunistic resources through the Notre Dame Center for Research Computing (CRC). Lobster grew out of an REU project, and there are still many exciting directions in which it could be further developed from making Lobster more intelligent so that it can automatically adjust to changing to taking Lobster beyond ND's campus to run on computers around the world.

47. (MDAPP) Modern Data Analytics Approaches in Particle Physics

Description:
Finding evidence for new particles in the data collected at the Large Hadron Collider (LHC) has been likened to finding a needle in a needle-stack. The particle physics community has developed computational tools to tackle this enormous challenge, and while the tools do an outstanding job of sifting through gigantic piles of data, they start to bog down during the final stages of analysis where quick turn-around time becomes critical. However, companies like Google have developed solutions that can search through data with lightning speed. In partnership with researchers at Hewlett-Packard, the REU student will explore the potential of the HP Vertica Analytics Platform to accelerate analysis of data from the Compact Muon Solenoid (CMS) experiment at the LHC.

48. (CLAD) Classification in Large Astrophysical Databases

Description:
Astrophysics is transitioning from an era when researchers would go to a telescope to get a couple of nights of data on a handful of targets to one in which they perform large-scale surveys that are the equivalent of thousands of nights on a single telescope. The Sloan Digital Sky Survey (SDSS) was the forerunner, leading to discoveries that were inconceivable at the time and continues to blaze new trails today. This REU project which focuses on sources within the SDSS that have shown variability in their brightness, such as matter accreting onto supermassive black holes in the center of galaxies. When sifting through the enormous volume of data from tens of thousands of sources, the problem is how to sort out the ordinary (red dwarf flare stars) from the extraordinary (comets and asteroids falling on to white dwarfs). REU students will develop software to classify sources and flag those that appear unusual.

49. (EAIG) Exploitation of Astrophysical Imaging within the Galaxy

Description:
Astrophysicists can learn a tremendous amount about the Universe by studying the details of the light spectra emitted by stars. For example, we can learn about how the elements in the Universe were produced or discover

details about how our galaxy came into being. The trick is to make detailed measurements of exactly the right stars from among the billions of possibilities. We are working on a new approach that uses data from Earth-based observatories that can scan large regions in the night sky and space-based observatories capable of capturing the entire sky. This data is not as detailed for any particular star as a dedicated observation, but it can be used to identify interesting objects for follow-up measurements. REU students will contribute to the development and testing of new techniques to identify the millions of important stars worth carefully measuring from among the 100 billion stars in the Milky Way. This is the first—and crucial—step towards the ultimate strategy of using large-scale sky surveys to help us find new sources of information for unlocking the secrets of the Universe.

50. (NMLAP) Novel Machine Learning Approaches in Physics

Description:
Over the past two decades, machine learning has become an established tool in physics. However, recent advances in other fields, such as image recognition or natural language processing have yet to be fully exploited within physics. For example, deep learning techniques first explored for image recognition have generated significant improvements over more conventional approaches within experimental particle physics. Another distinguishing factor for deep learning is the need for GPGPU programming techniques to accelerate the training process. REU students in both astrophysics and experimental particle physics will explore the potential for deep learning techniques when applied to research problems in those domains.

Projects with a Biology Focus

51. (CG) Computational Genomics

Description:
Sequencing technologies are transforming modern biology into a computational science. In the Notre Dame Bioinformatics Laboratory, we use large scale computation to extract understanding of biological functions from the gigabytes of data that describe an organism's DNA. Prior knowledge of biology is optional, but you should be willing to work in a team with diverse experience and research interests (including others in CS at ND, in the U.S., and abroad). We continue to be on the leading edge of genomics-focused technologies, and have multiple projects available ranging from traditional software development (C/C++/Java), algorithm research, to building cloud-enabled frameworks in collaboration with the ND Cooperative Computing Lab (CCL) and others. Potential implications of CS research include helping decipher important malaria mosquito genomes obtained from sub-Saharan Africa samples, detecting current and ancient (fossil) DNA from lakes, and predicting drug tolerance from clinical isolates of malaria.

52. (TRAITS) Identifying Bacteria Ecological Syndromes and Tradeoffs through Comparative Genomics

Description:
Bacteria can be found everywhere, from hydrothermal vents at the bottom of the ocean to your belly button. These microorganisms drive global biogeochemical cycles and may even drive your food cravings. Recent advances in DNA sequencing technology have provided access to the genome sequence of more than 40,000 bacterial species. In this project, students will work to identify genome-derived clues for where these bacteria live and how they make a living.

53. (HYDRO) Coupled Hydrologic and Biogeochemical Modeling of Lake Regions

Description:
Lakes and reservoirs are defining components of most landscapes globally. We also know that these ecosystems play an important role in regulating global climate change because they are hotspots for storage of carbon and release of greenhouse gases. Unfortunately, lakes and reservoirs are not currently included in the models used to predict future climate. Students working on this project will assist Notre Dame scientists in building the next generation of global models of climate change.

54. (EVGR) Epigenetic Variation and Gene Regulation.

Description:
Despite the significant amount of information on genetic variation, clear causal links between genetic variation and the onset of complex phenotypes including human disease are often elusive. In large part, this difficulty in linking genetic factors to phenotypes is due to complex genotype x environment interactions. Increasing evidence suggests that epigenetic factors often play a crucial role in mediating genotype x environment interactions that ultimately trigger the onset of diseases such as cancer and arthritis as well as contributing to cellular senescence. We are using next-generation sequencing in a model system, the waterflea Daphnia, to elucidate the role of epigenetic variation in modulating the patterns of gene regulation in response to environmental stress. The REU student will map epigenetic patterns in natural populations to reference genomes and RNA-seq data to test hypotheses about the relationship between methylation and gene regulation. Identifying bacterial ecological syndromes and tradeoffs through comparative genomics. The availability of bacterial whole genome sequences has grown exponentially over the last decade. Today, greater than 40,000 genome sequences are available in public databases. The field of microbial ecology is no longer data limited, and the challenge that faces the field now is how to most efficiently translate this data into ecological knowledge. The strategy this group has adopted is to combine comparative genomic approaches from microbiology and computer science with a trait-based ecological framework most often employed in plant ecology. In this project, we use machine-learning approaches to identify genomic markers of known ecophysiological traits of bacteria. Following the generation of these genomic traits, we can evaluate whether correlations exist between a suite of genomic traits, which would indicate ecological tradeoffs or syndromes. Additionally, associations between genomic traits and the distribution of bacterial through space and time can be evaluated. This general area of microbial trait-based ecology is rich with opportunities for summer students with interest in computer science or computational biology.

55. (MALARIA) Modeling Malaria Drugs using Genome-wide Transcriptional Response Profiles

Description:
Malaria is a global health concern, with over 200 million infections a year and 600,000 deaths. Through the use of drug treatment and vector control, malaria mortality has decreased 45% over the past decade. High-throughput drug screens have identified thousands of compounds with anti-malarial activity, however more research is needed to prioritize compounds for advancement into pre-clinical and clinical trials [37]. A large-scale methodology is needed to identify the mechanism of action (MOA) by which each of these drugs function to kill malaria parasites. We are developing methods to use transcriptional cellular responses of the deadly malaria parasite, Plas modium falciparum, to identify a set of genes and a pattern of expression that typifies a response to

perturbation by a particular drug (a signature of MOA). We hypothesize that the transcriptional response profile of P. falciparum to drug perturbation is highly indicative of the intracellular tar- gets of those drugs within the parasite and that the information can be used to predict drug MOA when the response profile for an unknown drug is compared to the response profiles for drugs with known MOA. A MOA signature for a given drug consists of the RMA normalized expression value for each gene normalized by the mean expression value across all perturbations for each gene. This normalization procedure removes the non-specific stress responses of the parasites and is a critical step for the successful application of our method. In this way we can build a database using the MOA signature for the drugs with known MOA to identify target relationships for drugs with no known target. Specifically, we need to demonstrate that drug perturbations in P. falciparum have a discernable MOA signature, build a reference database of MOA signatures, and validate the MOA signature using genetic perturbations [39, 40]. Finally we must show that the signature of an individual drug perturbation is consistent across experiments. We anticipate building a web tool to house the MOA signature database and allow queries for candidate drugs.

56. (CHROMO) Chromosome Inversions and Adaptation

Description:
The REU student will be involved in performing computer simulation models of how inversions (stretches of chromosomes with reversed gene order relative to each other) may affect the potential for ecological adaptation and speciation to occur when gene flow is occurring between populations. This is a very highly debated issue on the field of speciation genomics and it is thought that the recombination reducing effects of inversions Generated from computer simulations of a two-deme model of ecological speciation. Transition from low (genic) to high (genomic) levels of divergence and reproductive isolation (A), distributions of allele frequency differences (B, E), linkage disequilibrium (C, F), and population subdivision, Fst (D, G). may help in the divergence of different set of adaptive genes, facilitating speciation. However, many conflicting results call this theory into question. The student will work to ascertain the parameter space when inversion could facilitate the speciation process and be involved in analyzing DNA sequence data from Rhagoletis pomonella (in collaboration with colleagues from the Univ. of Illinois, Rice University, the Univ. of Colorado, and Kansas State University) and Drosophila pseudoobscura (in collaboration with a research team at Duke University) fruit flies currently being generated to empirical test predictions of the inversion hypothesis.

57. (GENETIC) Developing High-density Genetic Maps in Non-model Systems.

Description:
Understanding the genetic basis of phenotypic variation is central to evolutionary biology and human disease research. A powerful approach to make the connection between genome phenotype relies on a statistical analysis of the relationship between variation in the genome and variation in the phenotype. These analyses are referred to as Quantitative Trait Loci (QTL) analysis. This type of analysis is fundamental to modern agriculture and human disease research. QTL analysis requires a well-resolved genetic map which until recently were extremely difficult to construct in any non-model species. Recent advances in high-throughput sequencing now make it possible to establish high-density genetic maps in many species of ecological and evolutionary relevance. The REU student will work with sequence data to develop genetic maps and conduct QTL analysis in species ranging from freshwater invertebrates like the waterflea Daphnia, to important agricultural pests like Rhagoletis fruit flies,

and long-lived hardwood trees in the Oak species complex. Coupled hydrologic and biogeochemical modeling of lake regions: Lakes represent key biogeochemical hotspots globally. Across the Holocene, lakes have stored twice as much carbon in their sediments as is currently sequestered in terrestrial biomass. In addition, lakes and reservoirs process about one-third of the nitrogen and over half of the carbon exported from the terrestrial landscape annually. Unfortunately, the geographic, climatic, and hydrologic context of lakes is completely ignored when generating these estimates. Rather, global rates of carbon burial or release to the atmosphere are derived from average observed rates multiplied by global lake area. We are developing computationally scalable, coupled catchment-lake models to capture important spatial and temporal heterogeneity in lake biogeochemistry and greenhouse gas cycling. With recent NSF support we are augmenting these models to capture long-term, lagged responses of catchment land use. REU students with computational interests would be ideal for developing and testing these catchment modules for our existing regional model and testing these models with existing data on lake hydrology and biogeochemistry using model data fusion approaches.

CSS – Computational Social Science

Projects with a Computational Psychology Focus

58. Model fitting, model comparisons, and model selection uncertainty

Description:
Comparing multiple alternative models fitted to the same data has become one of the most popular approaches of behavioral data analysis. As models have become increasingly complex and more highly parameterized, the number of alternative models can be substantial. The usual strategy is to select a single "best-fitting" model, and interpret that model. In a recent paper we have shown that it is important to quantify how likely it would be that this model would be selected again in a new sample. In other words, we need to know how likely it is to replicate the results. If that chance is high then we can be more confident interpreting the results of a model fitting analysis than when that chance is small. To quantify this probability a large scale bootstrap procedure is required. As a summer project you would learn the basics of fitting models to psychological data on a computer cluster, and you would work together with graduate students to develop and test an R-package that carries out the model comparisons, the selection of the best model, and the computation of the model selection probability. The goal is to publish a paper that describes the package with a number of illustrative analyses.

59. Bayesian Analysis of Large-scale Complex Educational Data

Description:
This research involves analysis of large-scale cognitive and educational data from national studies and surveys. These data often have hierarchical or multilevel structures with missing data and non-normal data. Therefore, computationally intensive methods, such as Markov chain Monte Carlo methods, bootstrap and multiple imputation, have to be used to deal with the complexity of the data. One of the research questions that this professor is currently interested in is how mathematical ability and reading ability interplay with each other through the analysis of data from the Early Childhood Longitudinal Study, Kindergarten Class of 1998-99 (ECLS-K). There are significant amounts of missing data in this study and the data are not normally distributed. This

group has developed advanced statistical models utilizing Markov chain Monte Carlo based Bayesian methods to deal with such complex data. Better policy, therefore, can be developed to improve national education of mathematics.

60. Data Mining Large-scale Educational Assessment Data

Description:
This project's primary research interest lies in data mining on large-scale educational and psychological assessment data, such as, the Trends in International Mathematics and Science Study (TIMSS) data from over 60 countries, with about 4,000 participants in each country answering questions about their knowledge on math and science. This requires sophisticated statistical models to account for sampling characteristics, missing data, the multilevel structure in the data (i.e., participants nested in classes, classes nested in schools, and schools nested in countries), and linking and scaling (as the TIMSS runs a 4-year cycle).

61. Intelligent Tutoring

Description:
This professor's research interests are in the areas of human-computer interaction and human-robotic interaction. He is currently participating in three interdisciplinary teams which investigate the use of gaming technology (software and hardware) and interactive humanoid robots for such diverse research application as moral psychology, stroke rehabilitation/balance studies and autism therapy. He is collaborating with an international team of researchers to study moral decision making of remotely piloted aircraft (RPA), or drone pilots, utilizing a 3D video game simulation he developed. In the military scenario, participants fly the drone using a joystick and are faced with moral dilemmas similar to the classic trolley dilemma where they must choose between killing an individual or a group of five. Considerable data is collected throughout the experiment, such as psychology survey measures before and after the simulation, heart rate data during the simulation and time stamped events during the course of the simulation.

Projects with a Computational Sociology Focus

62. Interdisciplinary Center for Network Science & Applications

Description:
The NetSense (NSF) and now the NetHealth (NIH) project generate huge amounts of call detail records (CDRs) used to map social networks. For example, in the NetSense study over 70 weeks 160 students generated 23 million communication events yielding over 46,000 weighted edges in the network graph. The NetHealth project has increased the data quantity as we are collecting CDRs from 500 students and in addition health data (heart rates, sleep traits, steps) from all these students. Graduate students use the Computational Social Science Computer Cluster resources to match data records, anonymize data, compute network graphs and visualizations and construct overtime communication profiles for network social ties.

63. Racial, Economic, and Institutional Disparities in Home Mortgage

Description:
American homeownership has long been characterized by racial, ethnic and geographic inequality. Inequality in homeownership, in turn, has contributed to racial and class segregation and inequality in other aspects of American life. For several years, ND faculty has been examining the causes of this inequality in a project entitled Racial, Economic and Institutional Disparities in Home Mortgage Lending. In particular, the project looks at how characteristics of financial institutions and government policies affect lending to low income and minority markets. Funded by Department of Housing and Urban Development and the NSF, this research has gradually evolved from a small community service project into studies of St. Joseph County, the state of Indiana, and, most recently, the entire nation. This work has shown how the Community Reinvestment Act, the rise of subprime lenders, and the activities of the Government Sponsored Enterprises Fannie Mae and Freddie Mac affected lending to low income and minority groups during the 1990s and early 2000s.

Projects with a Computational Economics Focus

64. Large Overlapping Generations Models of Household Saving

Description:
This research involves international macroeconomics and finance, with a focus on understanding the evolution of the household saving rate in China, Japan, and the U.S. over time. To do this, this group needs to solve both closed and open economy versions of large scale overlapping generations models. These are dynamic economies that are populated by many agents differentiated by age, each of whom are solving individual lifetime utility maximizing problems by dynamic programming methods. The research team seeks the answers to two main questions. First, what is the role of the changing age distribution of the population? The second question is, what is the role of the precautionary saving motive?

65. General Equilibrium Structural Models and their Potential to Evaluate the Effects of Government Policy

Description:
This professor's primary research fields are industrial organization and international trade. He is particularly interested in quantifying the dynamic effects of government policy on firm and consumer decisions. The type of research questions of interest require solving complex models in which heterogeneous agents (firms and consumers) make strategic decisions (e.g., innovation, investment, consumption) conditional on their beliefs about the actions of other agents (including government). This amounts to solving high-dimensional and computationally-intense fixed-point problems both when generating equilibrium actions in the model consistent with the data and when evaluating equilibrium responses to changes in government policy.

Projects with a Cyberinfrastructure (CI) for Social Sciences Focus

66. Digital Historical Architectural Research and Materials Analysis (DHARMA)

Description:
The DHARMA project is a multidisciplinary archaeological, anthropologic, architectural, and computer science research collaboration which focuses on documenting historic monuments and buildings around the world with the use of a Leica 3D laser scanner, a high-speed, long-range scanner ideal for projects that are difficult to document by traditional methods. The scanner provides researchers with the most field-efficient means of data collection. Recently, the team has also used 3D scanning to determine and monitor seismic effects on historic buildings and reconstruction processes of buildings with historical value. In partnership with CyArk, a non-profit organization that collects the most accurate 3D models of cultural heritage sites, stores them and provides them freely to the world, the University plans to further use the scanner to document endangered historic buildings such as those on UNESCO's world heritage list or the U.S. National Register of Historic Places. The scanner is also used as part of the School's Preservation and Restoration Concentration. The DHARMA team spent four weeks in India documenting some of the country's historic monuments including the Taj Mahal. Additionally, a team of School of Architecture faculty and students traveled to the Roman Forum the center of political, religious and judicial life in ancient Rome.

67. Social Computing and Modeling & Simulation of Complex Social Systems

Description:
CI technology focuses include social computing, scientific and engineering databases, eTechnology applied to science gateways, portals, hubs, simulation and modeling, and UAV Swarms. These research collaborations apply these cyberinfrasructure technologies to research on engineering virtual organizations (EVOs), malaria transmission, citizen engineering, disaster management, understanding open source software, and disease transmission. Funding for these projects comes from the NSF, NIH, and the Bill and Melinda Gates Foundation. The Madey lab has hosted 16 different undergraduate researchers over the last five years. A published research paper describing a project by an undergraduate student is available at: http://t.co/Q7JfTdUV3m

68. Science Gateways-A Single Point of Entry for Modeling and Analysis Tools Across Organizational Boundaries

Description:
The use of science gateways is increasingly important in marshalling documents, discussion, software tools, and databases, and generally supporting heterogeneous communities of inquiry. Science gateways may be designed as collaborative research environments tailored to social networks for various use cases, e.g., in economics. At the University of Notre Dame we are leveraging science gateways to more easily manage the communication of people and data resources for several undertakings, such as collecting and analyzing democracy data from around the world in the science gateway "Varieties of Democracy" or managing data related to peace accords throughout the world in the science gateway "Peace Accords Matrix". The focus of this work is on helping to build a science gateway for modeling and analysis tools for social, psychological, economic, or anthropological data, tools and workflows.

69. Global Open Simulator

Description:
Through an undergraduate service learning course, this project is leading a new research initiative to develop a high performance yet accessible, multi-scale, human well-being simulation tool on the scale of 7 billion humans. REU students participating in research on the Global Open Simulator (GOS) will study tradeoffs in social model complexity with computational performance limitations.

70. Multicriteria Decision Making in Social Problems

Description:
This project investigates decision theory and applies it to real-life situations in social approaches to communities on local, regional and national (policy) levels. It will help the REU students understand how to analyze decisions with multiple objectives. Examples and problems focus on such strategic applications as community resilience planning, local resource planning and management, and priority setting for social and health intervention planning. The participants will study not only quantitative criteria and objective setting, but also social and ethical ones (values), which play important roles in decision-making.