2nd Annual Postdoctoral Research Symposium
University of Illinois

Beckman Institute, University of Illinois at Urbana-Champaign
January 27, 2012

Organizers: Hongmei Li, Taras Pogorelov, Yekaterina Golubeva, Evelina Tapia, Koushik Ghosh

Sponsors: Beckman Institute, Graduate College, Engineering College, Chancellor’s Office, and Institute for Genomic Biology

Beckman Foyer near Auditorium and Room 1005: Registration
8:00 – 8:40 Registration and coffee
Posts up from 8:45 am to 6:30 pm

Auditorium: Opening remarks and Keynote address
8:45 – 8:50 Welcome - Society of Postdoctoral Scholars, Hongmei Li
8:50 – 8:55 Remarks - Postdoctoral Affairs Office, Alexis Thompson
9:00 – 10:00 Keynote - Prof. John A. Rogers
Materials and Mechanics for Bio-integrated Electronics

Auditorium: Talks, Session 1
Chair: Mary Laws
10:00 – 10:15 Mary Laws
Perturbation of Estrogen Receptor Signaling in the Hypothalamo-pituitary-ovarian Axis Leads to Ovarian Tumorigenesis in Mice (1.1)

10:15 – 10:30 Sunil Mathanker
Biomass Yield Estimation Using LIDAR and Load Cells (1.2)

10:30 – 10:45 Craig Yendrek
Comparing the Ozone Response of Five Agriculturally Important Legume Species (1.3)

10:45 – 11:00 James Sikes
Exploring the Evolutionary Loss of Regeneration: A Comparative Genomics Study in Planarians (1.4)

Beckman Foyer near Auditorium and Room 1005: Break
11:00 – 11:20 Break: Coffee, tea, water

Auditorium: Talks, Session 2
Chair: Christopher Jones
11:20 – 11:35 Christopher Jones
Memory for Intended and Enacted Behaviors (2.1)

11:35 – 11:50 Sharlene Denos
Illinois Researchers in Partnership with Science Educators (iRISE): A New Model for Training Science and Engineering Graduate Students in Education and Outreach (2.2)

11:50 – 12:05 Justin Olmanson
Wayfaring Toward Possibility: Methodological and Analytical Sideways Moves in Social Science Research (2.3)
12:05 – 12:20  Ilia Solov’yov  
*Magnetoreception Mechanisms in Birds: Toward the Discovery of the Sixth Sense (2.4)*

**Room 1005: Lunch**  
12:20 – 1:10  Lunch

**Auditorium: Talks, Session 3**  
Chair: Wei-Cheng Lee  
1:10 – 1:25  Wei-Cheng Lee  
*New Route to Superconductivity (3.1)*

1:25 – 1:40  Bernard Lidicky  
*Bipartizing Fullerenes (3.2)*

1:40 – 1:55  Narayan Chapagain  
*Comparison of Zonal Neutral Winds and EPBs Velocities Over Brazil (3.3)*

1:55 – 2:10  Benjamin Smith  
*Machine Listening: ART and the Intelligent Acoustic Interface (3.4)*

**Beckman Atrium: Poster Session**  
**Beckman Foyer near Auditorium and Room 1005: Break**  
2:10 – 4:00  Poster session (Posters up from 8:45 am to 6:30 pm)  
3:00 – 3:20  Break: Coffee, tea, water (parallel with the Poster Session)

**Auditorium: Talks, Session 4**  
Chair: Maksym Kryvohuz  
4:00 – 4:15  Maksym Kryvohuz  
*Calculation of Quantum Reaction Rates via the Instanton Approach (4.1)*

4:15 – 4:30  Michael Slater  
*Composite Sodium-Lithium-Transition-Metal Oxides as Cathodes in Alkali-Ion Batteries (4.2)*

4:30 – 4:45  Darya Radziuk  
*Ultrasonic Formation of Binary Gold-silver Nanostructures (4.3)*

4:45 – 5:00  Mahmoud Moradi  
*Inward-facing to Outward-facing Transition of GlpT Transporter, Studied Using Nonequilibrium Molecular Dynamics Simulations (4.4)*

**Auditorium: Closing Remarks**  
5:00 – 5:10  Closing remarks, Taras Pogorelov

**Beckman Atrium: Reception**  
5:15-6:15  Reception  
Best Talk award  
Posters are accessible
1.1 Mary Laws *Perturbation of Estrogen Receptor Signaling in the Hypothalamo-pituitary-ovarian Axis Leads to Ovarian Tumorigenesis in Mice*

Ovarian cancer is the most lethal malignancy of the female reproductive system. Due to the absence of strategies for early detection of ovarian malignancies, the majority of women with ovarian cancer are diagnosed at a late stage. We have developed a mouse model in which aberrant estrogen receptor alpha (ERα) signaling in the hypothalamo-pituitary-ovarian axis leads to ovarian tumorigenesis. In this mouse model, termed ERαd/d, a conditional deletion of ERα gene occurred in the anterior pituitary. Selective ablation of ERα in the pituitary created a systemic hormonal imbalance in these mice. The ERαd/d mice exhibited formation of ovarian tumors with 100% penetrance, starting at 5 months of age. The ERαd/d mice displayed an elevated ERα signaling in the surface epithelial cells of the ovary. We observed an elevation in the expression of phosphorylated ERα (at Ser-118) in the ERαd/d ovarian epithelial cells. Immunohistochemical analyses revealed that the cells within the ovarian tumors of ERαd/d mice are characterized by intense expression of cytokeratin 8 and nuclear staining of Wilms tumor 1. In summary, we have developed an animal model, which will serve as a powerful tool for exploring the involvement of ERα-dependent signaling pathways in the etiology of ovarian cancer.

1.2 Sunil Mathanker *Biomass Yield Estimation Using LIDAR and Load Cells*

Improving the efficiency of mowing and baling is one of the challenges to improve biomass supply logistics. Previous field evaluation results show large variations in field speed of forage equipment used for bioenergy crops. Currently, the operator controls the machine speed mainly based on his own judgment. It was hypothesized that a feed forward real time sensing system to measure incoming biomass might result in enhanced machine capacity. In this study a LIDAR sensor was mounted on the back of a forage harvester to measure the swath. Similarly, the Load cells were mounted on the front of a forage harvester to measure the incoming biomass. The sensing system was evaluated for switch grass, prairie grass, and miscanthus. The sensed data was correlated to biomass yield and field locations. It is expected that integration of real time biomass estimation could improve efficiency of existing machinery and could be useful in many other precision agriculture applications.

1.3 Craig Yendrek *Comparing the Ozone Response of Five Agriculturally Important Legume Species*

In the past 100 years, tropospheric ozone concentrations [O3] have more than doubled in response to industrialization. Current [O3] can cause oxidative damage in plants, leading to yield losses that have been estimated to cost growers $1.8-3.6 billion per year for soybean in the US. Models indicate that [O3] will continue to rise another 25% by 2050, thus exacerbating the strain on agriculture to provide food at a time of rapid population growth. Here, we compare the O3 response of Glycine max, Pisum sativum, Phaseolus vulgaris, Cicer arietinum and Medicago sativa - all commercially relevant crops, important for global food security. When grown in elevated O3, measurements of stomatal conductance (gs) revealed a broad range of O3 sensitivities. The most sensitive species, P. vulgaris and M. sativa, each had decreases in gs of 55%, while the most tolerant species, P. sativum, was not significantly different from ambient-grown plants. G. max and C. arietinum showed an intermediate response, with decreases in gs of 46% and 36%, respectively. To identify specific markers of O3 tolerance at the molecular level, we have undertaken a transcriptome sequencing approach using the Illumina platform to compare global changes in gene expression between these legume species.

1.4 James Sikes *Exploring the Evolutionary Loss of Regeneration: A Comparative Genomics Study in Planarians*

Planarians possess extraordinary abilities to regenerate complete animals from small tissue fragments. However, in contrast to most flatworm species, the planarian *P. fluviatilis* is limited in its ability to restore lost structures, failing to regenerate heads when amputated in posterior tissues. To identify the critical mechanistic failure in *P. fluviatilis* regeneration, we have compared the early stages of regeneration following amputation in tissues with different regeneration potentials. While the earliest regenerative phases, such as wound healing and cell proliferation, appear to occur normally in regeneration-deficient tissues, wnt/beta catenin and FGF signaling as well as the reestablishment of anterior-posterior polarity fail to occur. To examine and contrast global changes in gene expression at this critical time point, we have conducted comparative transcriptomic analyses using RNAseq. Genes upregulated in regeneration-proficient tissues yet
not expressed in regeneration-deficient tissues have been identified as candidates with putative functions important to the regeneration process. In an attempt to identify the permissive and/or inhibitory factors involved in planarian regeneration, we are determining the specific roles of these genes using RNA interference in P. fluviatilis as well as in the related regeneration-competent planarian Schmidtea mediterranea.

2.1 Christopher Jones Memory for Intended and Enacted Behaviors

We examined the potential of behavioral intentions to produce false memories of enacted behaviors, hypothesizing that in the case of easily-enacted behaviors, individuals would tend to mistake merely intended behaviors as enacted ones. Results of three experiments showed that behavioral intentions produced more false memories than a control condition across multiple operationalizations of intended and enacted behaviors.

2.2 Sharlene Denos Illinois Researchers in Partnership with Science Educators (iRISE): A New Model for Training Science and Engineering Graduate Students in Education and Outreach

I describe a program, Illinois Researchers in Partnership with Science Educators, iRISE, that represents a new model for training science and engineering PhD students in science education and outreach. iRISE is centered around a course which provides instruction in pedagogy, lesson development, assessment, diversity and other broad issues in K-12 education. The practicum part of the course involves teaching a one-hour lesson to underprivileged middle school students at a local community center. At the end of the semester, revised lessons are made available to educators via the program website and four lessons are disseminated to teachers during a summer workshop taught by a subset of graduate students from the course. We present findings from our evaluation of this program related to the impact on graduate student and middle school student participants. Our data indicates the program positively impacted graduate students communication skills and middle school students attitudes about science and engineering. We find that offering a graduate level course from within a scientific discipline provides a sufficient reward for a relatively short and unambiguous time commitment from time-strapped graduate students. In addition, the course provides a continuous source of mind and manpower for K-12 outreach and teacher professional development.

2.3 Justin Olmanson Wayfaring Toward Possibility: Methodological and Analytical Sideways Moves in Social Science Research

In this paper and presentation I outline several sideways moves available to researchers in the social sciences. The construct of a sideways move comes from the scholarship of anthropologist Kathleen Stewart. She writes of non-adversarial, non-paranoid methodological and analytical approaches that open up the possibility for a different, more performative mode of address in social science research. From this beginning I describe some of these approaches and situate them within the social sciences and educational research literatures. I after introduce New Ethnographic Writing, Non-Representational Theory, Weak Theory, and Actor-Network Theory I outline what they make possible as well as provide a few examples from my efforts to apply them in educational research.

2.4 Ilia Solov'yov Magnetoreception Mechanisms in Birds: Towards the Discovery of the Sixth Sense

Many animals are able to sense the Earth's magnetic field and use it for their orientation. Starting in the 1960s this magnetic sense was first described for higher organisms and later also experimentally shown for bacteria. The best investigated magnetic sense today is the compass of migrating birds. But even there, many details still elude the investigation. Most likely, the animal magnetic sense is based on two types of receptors, one containing tiny magnetic minerals, and the other one possessing reactive free radicals. I will discuss both mechanisms and present results of recent theoretical analysis aimed towards understanding the nature of the magnetoreception mechanism.

3.1 Wei-Cheng Lee New Route to Superconductivity

Superconductivity, electrical conduction without any loss below some critical temperature \( T_c \), occurs in numerous materials. This field began in 1911 with the discovery of superconductivity in mercury at 4.2K. After the birth of a complete microscopic theory of superconductivity proposed by Bardeen, Cooper, and Schrieffer in 1957, known as BCS theory, it was believed that no materials could have \( T_c \) higher than 30K. The discovery of new classes of superconductors, cuprates in 1986 (which shatter the 30K barrier) and iron pnictides in 2008, launched an international wave of research to find new materials with higher \( T_c \). In this talk, I will explore a new concept for route to superconductivity in which the key elements of the cuprates and iron-
based superconductors are combined. The hope is that such a concept could lead to our dream of room-temperature superconductors.

3.2 Bernard Lidicky Bipartizing Fullerenes

A fullerene graph is a cubic bridgeless planar graph with twelve 5-faces such that all other faces are 6-faces. We show that any fullerene graph on n vertices can be bipartized by removing O($\sqrt{n}$) edges. This bound is asymptotically optimal.

3.3 Narayan Chapagain Comparison of Zonal Neutral Winds and EPBs Velocities Over Brazil

We present the first simultaneous measurements of equatorial thermospheric neutral wind measurements and plasma bubble (EPB) zonal speeds over northeastern Brazil during September-December 2009 and 2010. The wind data are obtained from a bi-static Fabry-Perot interferometer experiment measuring the Doppler shift of the 630.0-nm spectral emission. The FPIs are located at Cajazeiras (6.86°S, 38.56°W) and Cariri (7.38°S, 36.53°W). The EPB zonal speed, which is assumed to be equal to the drift of the background plasma, is measured using images of the 630.0-nm emission obtained from a wide-angle imaging system collocated with the FPI at Cajazeiras. In general, the simultaneous measurement of the zonal neutral wind and the EPB zonal speed show excellent agreement. However, the EPB zonal speed is slower than that of the wind motion in the early evening hours on several occasions, suggesting the F-region dynamo is not fully activated.

3.4 Benjamin Smith Machine Listening: ART and the Intelligent Acoustic Interface

Recent developments in machine listening present opportunities for innovative new paradigms for computer-human interaction. Voice recognition systems demonstrate a typical approach that conforms to event oriented control models. However, acoustic sound is continuous, and highly dimensional, presenting a rich medium for computer interaction. Unsupervised machine learning models present great potential for real-time machine listening and understanding of audio and sound data. We propose a method for harnessing unsupervised machine learning algorithms, Adaptive Resonance Theory specifically, in order to inform machine listening, build musical context information, and drive real-time interactive performance systems. We present the design and evaluation of this model leveraging the expertise of trained, improvising musicians.

4.1 Maksym Kryvohuz Calculation of Quantum Reaction Rates via the Instanton Approach

Calculation of reaction rate constants is an important task of theoretical chemistry. The rate limiting-step of many chemically and biologically important processes is proton, hydrogen or hydride transfer reactions. Due to the light mass of the transferring hydrogen atom, nuclear quantum effects such as tunneling and zero-point energy may play a significant role. A modified version of the instanton theory have been recently proposed, which is capable to correctly describe nuclear quantum effects in multiatomic systems at arbitrary temperatures. The attractive feature of the instanton approach is its weak scaling with system size. The latter allows to calculate potential energy surface on the fly and makes the instanton approach a promising method that is capable to rigorously describe quantum reaction rates in systems of up to hundred atoms on the ab initio level. The approach is illustrated on several multiatomic systems.

4.2 Michael Slater Composite Sodium-Lithium-Transition-Metal Oxides as Cathodes in Alkali-Ion Batteries

Sodium-lithium-transition metal oxide composites find application as cathode materials in sodium-ion and lithium-ion electrochemical energy storage systems. Variations in the ratio of alkali metals affect the phase distribution of the composite, with lithium residing in Li-only phases and also appearing as a dopant in the transition metal plane of lamellar sodium oxides. Low temperature ion-exchange of Na by Li produces high-capacity lithium-ion cathode materials with extensive stacking fault defects. The influence of structural factors in these materials on electrochemical performance will be presented.

4.3 Darya Radziuk Ultrasonic Formation of Binary Gold-silver Nanostructures

Acoustic cavitation, which is the formation, growth and abrupt collapse of gas/vapour filled microbubbles, is used as a tool to design preformed gold nanoparticles with silver in water. The surface energy of bubbles is transformed into the thermal (hot gas phase interior ~ 103 K), mechanical (shock waves and turbulent jets) and chemical (radical formation) energy of water. We developed two ultrasonic approaches for formation of binary gold-silver nanoparticles in aqueous solutions of surface active additives (e.g. surfactants, alcohol or polymers). In the first method silver ions (silver nitrate aqueous solution) are reduced on the surface of the citrate-protected gold sols (25 7 nm), yielding binary gold-silver nano-worms. The other approach is based on
the sonication of preformed gold and silver nanoparticles in aqueous solution of surfactants. Cationic dodecyl amine coats the negatively charged metal surface and particles are adsorbed on the gas/liquid cavitation interface. Upon the bubble collapse gold and silver nanoparticles are transported into the hot gas-phase bubble interior yielding binary Au-Ag alloy nanostructures. This work provides pioneering results in fusion of nanoparticles with a pronounced Ostwald-like ripening effect (the less cohesive particles are transported towards the most cohesive) during acoustic cavitation.

4.4 Mahmoud Moradi Inward-facing to Outward-facing Transition of GlpT Transporter, Studied Using Nonequilibrium Molecular Dynamics Simulations

Glycerol-3-phosphate transporter (GlpT) is a member of major facilitator superfamily (MFS), the largest family of secondary transporters. Similar to other transporters, GlpT is believed to function using an alternating-access mechanism during which it undergoes large conformational changes. The only available structure of GlpT is in the apo inward-facing (IF) state. In our earlier work using equilibrium molecular dynamics (MD) simulations, the binding site of GlpT was characterized and the initial substrate-induced closing on the cytoplasmic side was observed. Here we have used a novel approach based on nonequilibrium MD simulations to drive the transition of GlpT from its available IF state to its unknown OF state in an explicit membrane environment. A set of non-conventional collective variables were defined for the transmembrane helices to specifically reflect the conformational changes involved during the IF-to-OF transition. The system was then steered along these collective variables in a nonequilibrium scheme. Nonequilibrium work relations were used to analyze the trajectories and extract information about the OF state structure, the IF-to-OF transition mechanism, and the characteristics of the OF-state binding site, providing insight about the general mechanism of MFS transporters and more generally introducing a novel approach to study the IF-to-OF transitions in membrane transporters.

**Posters**

For a complete list of co-authors please see the posters

5.1 Thomas Garcia Constitutive expression of activated NOTCH1 in fetal Sertoli cells leads to premature gonocyte differentiation

5.2 Yekaterina Golubeva Integrating Global Regulatory Input into the Salmonella Pathogenicity Island 1 Type III Secretion System

5.3 Arindam Chakraborty Phosphorylation of Orc6 and HP1 by NDR kinases is crucial for cell cycle progression

5.4 Vidisha Tripathi Role of SR splicing factors in nuclear speckle organization and gene expression

5.5 Taras Pogorelov Glycophorin A transmembrane helix insertion, positioning and dimerization in model membranes

5.6 George Glekas The Bacillus subtilis Chemoreceptor McpC Senses Multiple Ligands Using Two Discrete Mechanisms

5.7 Hanna Walukiewicz Attractant binding induces changes in the polar and lateral chemotactic receptor clusters in Bacillus subtilis

5.8 Courtney Sloan Investigating Protein-Lipid Binding via Lipid Bilayer Nanodiscs Immobilized on Silicon Photonic Optical Microring Resonators

5.9 Suk Jin Ha Engineered Saccharomyces cerevisiae capable of simultaneous cellobiose and xylose fermentation

5.10 Melikhan Tanyeri Confinement and manipulation of micro and nanoscale particles with fluid flow

5.11 Nobuhiro Yanai Self-Assembly of Polyhedral Colloids
5.12 **Chandra Nath** Performance Evaluation of an Atomization-based Cutting Fluid Spray System in Turning of Titanium Alloy

5.13 **Manoranjan Sahu** Organic Catalysts in Promoting CO2 Absorption in a Hot-Carbonate Process Enabled with Crystallization for Post-combustion CO2 Capture

5.14 **Yonghong Zou** Validating and Optimizing Determination of Glyphosate and AMPA by LC-UV and LC-MS/MS

5.15 **Yanxin Liu** Protein folding thermodynamics and kinetics from all-atom molecular dynamics simulations

5.16 **Ning Shen** PARAMCHEM: Automatic Forcefield Parameterization Tool

5.17 **Qiong Cheng** Towards An Integrative Systems Biology Tool for the Exploration, Analysis, and Comparison of Dynamic Biological Networks

5.18 **Hongmei Li** Aggression and Metabolism in Drosophila and Honeybees

5.19 **Monica Elmore** Direction learning in a spatial T-maze task by neonatal piglets

5.20 **Michelle Green** Sensitivity of sampling tools used to detect chronic wasting disease in Illinois

5.21 **Aminda O’Hare** MAOA, Trait Anxiety, and Interference on an Emotional Flanker Task

5.22 **Simona Buetti** Impact of illusory control on time perception in normal and spider-fearful individuals

5.23 **Blake Jones** Daily Routines of Children with Asthma: Using Daily Diary Methods to Study the Health and Well-Being of Children with Chronic Asthma and Their Parents

5.24 **Vance Martin** Re-Envisioning Teacher Education at the University of Illinois

NOTES
Vote for the Best Talk
Please check **three** talks you enjoyed most

**Session 1**
- **10:00 – 10:15** Mary Laws
  *Perturbation of Estrogen Receptor Signaling in the Hypothalamo-pituitary-ovarian Axis Leads to Ovarian Tumorigenesis in Mice (1.1)*
- **10:15 – 10:30** Sunil Mathanker
  *Biomass Yield Estimation Using LIDAR and Load Cells (1.2)*
- **10:30 – 10:45** Craig Yendrek
  *Comparing the Ozone Response of Five Agriculturally Important Legume Species (1.3)*
- **10:45 – 11:00** James Sikes
  *Exploring the Evolutionary Loss of Regeneration: A Comparative Genomics Study in Planarians (1.4)*

**Session 2**
- **11:20 – 11:35** Christopher Jones
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**Session 4**
- **4:00 – 4:15** Maksym Kryvohuz
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  *Inward-facing to Outward-facing Transition of GLpT Transporter, Studied Using Nonequilibrium Molecular Dynamics Simulations (4.4)*
Symposium Feedback Form

We appreciate your feedback and look forward to your participation in future events

What aspects of the symposium were most useful?

What aspects of the symposium were least useful?

What additional sessions do you wish to see in the future symposia?

What is your overall rating of the symposium? If your reply is below excellent/good, please suggest ways to improve future symposia

☐ Excellent  ☐ Very Good  ☐ Good  ☐ Fair  ☐ Poor

How did you learn about this event?

☐ Society of Postdoctoral Scholars mailing list  ☐ Friends  ☐ SOPS website
☐ Postdoc Affair Office email  ☐ Other: __________________________

Which career paths/topics you would like to be covered in future SOPS events?

☐ Academic career  ☐ Industry career  ☐ Government career  ☐ Other: __________________________

What are the best times for you to attend events? Check all that apply.

☐ 12 – 3 pm  ☐ 3 – 5 pm  ☐ 4 – 6 pm  ☐ 5 – 7 pm  ☐ Other: __________

We welcome any additional feedback or comments

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Thank you!