Compiled Abstracts

22 April 2010
Student Center Grand Ballroom
Colorado School of Mines
Schedule of Events for April 22nd, 2010
Ben H. Parker Student Center Grand Ballroom
20th Annual GSA Research Fair

7:30-9:00 AM. Check-in and setup of posters.

9:00-11:00 AM. Morning poster session.
   (posters demarcated by gold tags)

11:00-12:30 PM. Lunch in the Coolbaugh Hall Atrium.

12:30-2:30 PM. Afternoon poster session.
   (posters demarcated by blue tags)

2:30-3:30 PM. Intermission.

3:30-3:45 PM. Awards reception with cheese, crackers and wine.

3:45-5:00 PM. Awards Presentation.
20\textsuperscript{th} Annual GSA Research Fair

Ben H. Parker Student Center Grand Ballroom

2009-2010 GSA Officers

President ~ Dan Baker

V.P. of Communications ~ Zach Aman

V.P. of International Students ~ Juan Carlos Carratu

Treasurer ~ Josh Lau

Academic Chair ~ Eric Chandler

Social Chairs ~ Stephanie Carr, Andrea Ham

We want to give our utmost gratitude to the volunteer and honorary judges, for their time and effort in making the 2010 GSA Research Fair a tremendous experience!
List of Abstracts – Morning Session

The Molecular Hubbard Hamiltonian ................................................................. 10
A Statistical Shape Model for Probabilistic Studies of the Lumbar Spine ................ 11
Robust Optimization of NURBs Metamodels for Engineering Design .................. 13
Phosphonic Acid Based Copolymer Fuel Cell Membrane .................................. 15
Operation of Solid-Oxide Fuel Cells under Biogas Fuel Streams ......................... 18
New Route to Sulfonic Acid Functional Polymers ............................................... 20
A Systematic Approach to Tubular SOFC Stack System Identification and Control based on LPV Model Structures and Model Predictive Control ........................................ 21
Microbial Diversity Associated with Single Cell Protein Produced from a Brewery Wastewater Pilot Plant ................................................................................................. 22
Joint Denoising of a Signal Ensemble: the Power of Veto .................................... 24
Quantum Many-body Tunneling of Bose-Einstein Condensates ............................ 25
Predicted response of microstructure, distortion, and residual stress in carburized steels cooled via oil and high intensity quenching ......................................................... 26
Microstructure-Mechanical Property Relationships for Ni-Ti-Pt High Temperature Shape Memory Alloys ................................................................................................. 27
The Microstructural Response of 1045 and 4145 Steel to Induction Hardening ........ 28
Hydrogen Peroxide Dynamics in an Agricultural Headwater Stream: Evidence for Significant Biological Production ................................................................. 29
Near Real Time Sensing of Uranium Contamination using Wireless Sensor Networks .... 30
Using Circuit-Level Power Measurements in Household Energy Management Systems .... 31
Technique for Large-Scale EBSD Mapping of Polycrystalline Silicon .................... 32
Ionic hybrid nanostructures for energy conversion ............................................... 33
Constructing Rigorous MANET Simulation Scenarios with Realistic Mobility ........ 34
Mineralogy and its contribution to anisotropy and kerogen stiffness variations with maturity in the Bakken Shales .............................................................................. 36
The Transformation of the U.S.-ROK Alliance: Balancing American Strategic Flexibility and South Korean Modernization ............................................................... 37
Polymer Modification of Nanoparticles for Controlled Morphology of Nanoparticle/Polymer Films .......................................................................................................... 38
<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to Build a Tricorder: Developing a Quantitative Habitability Prediction Tool for Planetary Exploration</td>
<td>39</td>
</tr>
<tr>
<td>TestbedProfiler v2: An Improved Validation Tool for Wireless Sensor Network Testbed Deployment</td>
<td>41</td>
</tr>
<tr>
<td>Solution Deposition of Amorphous IZO Films by Ultrasonic Spray</td>
<td>42</td>
</tr>
<tr>
<td>Lifespan of Horizontal Wick Drains</td>
<td>43</td>
</tr>
<tr>
<td>Microbial and Substrate Characterization of Four BLM Biochemical Reactors in the Coeur D’Alene Idaho Area</td>
<td>45</td>
</tr>
<tr>
<td>Study of Microalloy Precipitation in Hot Charged Slabs</td>
<td>46</td>
</tr>
<tr>
<td>Solution Processed NiO Modified Anodes in Bulk Heterojunction Organic Solar Cells</td>
<td>47</td>
</tr>
<tr>
<td>Quasiparticle Spectrum of 2-d Dirac Vortices in Optical Lattices</td>
<td>48</td>
</tr>
<tr>
<td>Predictive Bio-Computational Wear Modeling for Joint Replacements</td>
<td>49</td>
</tr>
<tr>
<td>Development of a Directionally Independent Roller Measurement Value</td>
<td>52</td>
</tr>
<tr>
<td>A Model for the Envelopes of Spin Waves in Magnetic Film Feedback Rings</td>
<td>53</td>
</tr>
</tbody>
</table>
List of Abstracts – Afternoon Session

Analysis of Trace Organic Contaminants in Raw Wastewater at various sewershed scales by Liquid Chromatography-Tandem Mass Spectrometry ................................................................. 56

Static Reservoir Modeling in an Incised Valley Fill: A Case Study in Optimization from Postle Field, Texas County, Oklahoma ................................................................. 58

Rheology & Chemical Characterization of Alaska Heavy Oils ................................................................. 60

Electrochemical Behavior of Titanium and its Alloys in Simulated Body Fluid ........................................... 63

Hydrogen Storage in Clathrate Hydrates: Unlocking Energy From Icy Cages ............................................. 64

Determining a Rheological Protocol for Measuring the Fluid Properties of Bio-oil ................................. 66

Microbial preservation potentials in a silicifying hot spring in Yellowstone National Park: experimental and in-situ examination from living to lithified ................................................ 67

Gas Transport and Internal-Reforming Chemistry in Solid Oxide Fuel Cell Anode Materials and Structures ........................................................................................................... 69

Predicting Intrinsic Damping of Soil Using Micro-Scale Tests ................................................................. 71

Optimization of connections between feeders in an emerging distribution system ............................... 72

Assessing DNAPL dissolution kinetics a bench-scale fracture network ....................................................... 73

Combined Lidar-based feedforward and feedback controllers for wind turbines with tower and blade damping .................................................................................................................................. 74

Locating abandoned coal mines to assess subsidence risk using self-potential and DC resistivity, Weld County, Colorado ........................................................................................................... 77

Hole Cleaning using “Conventional and Enhanced Sweep” ........................................................................ 79

Heap Leaching: A New Approach to Uranium Mining Waste Utilization .................................................. 80

Fault Tolerant Linear Algebra: Recovering from Fail-Stop Failures without Checkpointing .................. 82

Reconstructing the Sedimentary Deposits of Arabia Terra, Mars ............................................................ 84

Engineering band gap and conductivity of Ga : Zn_{1-x} Mg_x O by Pulse laser deposition .......................... 86

Model Reference Adaptive Control of Discrete Repetitive Processes in the Iteration Domain .. 87

Design and Implementation of a Remote Control System for Teleoperation of a Skid-Steer Loader over a Wi-Fi Mesh Network ........................................................................................................... 88

Performance of Alcohol Fueled Micro-Tubular SOFCs ........................................................................... 89

Applying Heavy Oil Geochemical Composition and Physical Properties in Determining Production Methods ........................................................................................................... 90

ADMIRE: Autonomous Dam Monitoring with Integrated Real-time Evaluation .................................. 91

Cooperative Beamforming: Higher Throughput with Collisions ................................................................... 92
Intelligent and Continuous Performance Monitoring: Impacts To Dam and Levee Safety Policy

A Dynamic Graph-Based Systems Framework for Modeling, of Cyber-Physical Systems Typified by Buildings

Surface Reaction Mechanisms during Ozone and O₂ Plasma Assisted Atomic Layer Deposition of Aluminum Oxide

Soliton Dynamics of a Line Vortex Defect Embedded in an Incompressible Inviscid Fluid


Polymer Modification of Nanoparticles for Controlled Morphology of Nanoparticle/Polymer Films

Biologically enhanced DNAPL dissolution kinetics within bench-scale experimental bedrock fractures

Coal Pre-treatment and its Effects on Extractable Organic Matter

Building and Adding Value to a Geothermal Academy: Microbial Fuel Cell Bioengineering & Collaboration with Icelandic Biogeothermal Resources

Acoustic impedance inversion for static and dynamic characterization of a CO₂ EOR project, Postle Field, Oklahoma

Microsecond simulations of spontaneous gas hydrate nucleation and growth
Morning Poster
Session Abstracts
We present the Hyperfine Molecular Hubbard Hamiltonian (HMHH), which describes an ultracold gas of heteronuclear alkali dimer molecules loaded into an optical lattice. A strong DC electric field orients the molecules, giving rise to long-range dipole-dipole forces and allowing for transitions in an AC microwave field. A strong magnetic field orients the nuclear spins. Together these fields allow dynamical control over the timescale and number of states involved in dynamics. We discuss three of the HMHH's experimental consequences: quantum dephasing, the dependence of the phase diagram on the molecular state, and tunable complexity, and provide characteristic entangled quantum dynamics simulations.
A Statistical Shape Model for Probabilistic Studies of the Lumbar Spine

Introduction:

Computational modeling of the spine has become a promising option for evaluating the performance of new spinal implants and procedures before they are used in patients. Most models in the literature only represent a single subject and neglect normal variation that exists between specimens. However, using a probabilistic simulation (select input variables from a normal distribution and determine how they affect outputs) of virtual patients, whose geometries are representative of actual patients, may lead to viable options for pre-clinical evaluation of devices and procedures. One of the major challenges to overcome when applying probabilistic modeling techniques to biologic systems is to capture normal shape variation between subjects.

Methods:

Vertebral body geometries from 8 normal CT scans were used to develop a statistical shape model (SSM) of the lumbar spine. The SSM model is comprised of eigenvalues and eigenvectors calculated with a principle component analysis. Eigenvectors, also called modes, represent how shape varies in the geometry and eigenvalues represent how important each mode is to the overall shape of the geometry. Any specimen can be represented by $P = P_{mean} + \sum_{j=1}^{m} b_j \cdot c_j$ where $b_j$ are scalar coefficients and $c_j$ are the eigenvectors. Virtual specimens can be created by randomly sampling the normal curve for each $b$ coefficient.

A finite element model, shown in figure 1, was developed containing eight ligaments (non-linear springs), an intervertebral disc, and transverse processes identified.

Figure 1: Finite element model of lumbar spine with ligaments (green), disc (red), cartilage (blue), and transverse processes identified.
(hyperelastic annulus, fluid cavity for nucleus), and linear elastic cartilage (2mm thick). A compression load of 800 N and 7.5 Nm of axial rotation was applied to the model and it was solved using Abaqus. The model was validated using experimental range of motion data.

For the purpose of probabilistic analysis, tens to hundreds of model runs are desired. To facilitate the generation of these models, a procedure was developed to incorporate geometry from the SSM, automatically place ligaments and generate cartilage.

**Results:**

The first mode shape was a scaling mode, the second was associated with shape and angulation of the facet joints and the third produced variations in transverse processes. Higher modes were not visually obvious. Models created from virtual geometries demonstrated noticeable shape variation but they mated quantitatively similar to models generated from CT scans (naturals). Qualitatively, differences between virtual specimens and natural specimens were not statistically different for either area or average pressure. For manual and automatic cartilage, contact area was observed in the same general location and contact pressure was similar, 2.43 MPa compared to 2.22 MPa.

**Discussion:**

Shape variation in the lumbar spine was characterized using a statistical shape model. Models created with virtual specimens demonstrated facet contact similar to models generated with natural specimens. Cartilage generation that was automated for a probabilistic study resulted in quality meshes that fit flush into the facet geometry.

With the success of models developed using virtual specimens, the same methods can be applied to the entire lumbar spine. Next steps for creating a probabilistic model are to automate the alignment of vertebral bones and implementation of probabilistic computations using a Monte Carlo method.
Robust Optimization of NURBs Metamodels for Engineering Design

Name: John C. Steuben
Degree Program: MS
Department: Engineering
Advisor: Dr. Cameron J. Turner

Engineering design is generally characterized as an activity where a designer compares alternative solutions to an engineering challenge in order to meet some required level of performance. Almost invariably this involves the selection of values for design variables such that the design meets performance requirements. Unfortunately, in many modern engineered products and systems the number of these design variables exceeds what an engineer may comfortably contemplate using traditional tools. Optimization tools which allow engineers to quantify and maximize performance in high-dimensional design spaces will become increasingly indispensable to the engineer if they can perform two tasks. These tools obviously must be able to search the design space for design variable values that maximize performance. Simultaneously, they must locate and quantify designs that provide robustness, or insensitivity in performance with respect to uncertainty or variation in design parameters. The considerations of modern manufacturing and control systems force this second requirement, as no machine component can be produced without variation, nor can any system be controlled with arbitrary accuracy.

When optimizing a design, a common difficulty is encountered. Many, if not most, engineering challenges are represented by system models of great complexity. Adequate analysis and optimization of the model is subsequently impossible due to time and computation limitations. As a result, surrogate models termed “metamodels” are used in place of the actual system model. These metamodels are far more computationally efficient and allow the optimization of otherwise intractable problems. Non-Uniform Rational B-Splines (NURBs) have emerged as a powerful metamodeling technique capable of addressing the twin challenges posed above. Previous research has resulted in the development of algorithms capable of fitting NURBs metamodels
to design spaces of many input variables and performance indices, and performing various discreet optimizations upon these metamodels. In the present research we expand upon this basis by illustrating the development of robust optimization algorithms that leverages the unique properties of NURBs metamodels. This optimization is conducted in a general fashion by considering both optimality and various robustness metrics as global or local model properties, and illustrates the tradeoffs between them using a novel graphical approach.
Advances in fuel cell membranes are needed for commercialization to be realized. These advances need to be made in many areas including mechanical durability, chemical resistance and increased power density. However, advances in the first two areas need to be accompanied by an increase in power density, in which the underlying problem is the rate of ionic transport. There are two main ways to increase transport; increase the hydration within the membrane to increase proton transfer via the vehicle mechanism or to increase the acidity of the polymer by using super-acids or increasing the number of acidic groups present. Since there are many benefits to being able to run under hot, dry conditions, the second approach is more acceptable for designing a new copolymer system.

In this work, zirconium divinyl phosphonate (VZP) has been copolymerized with vinyl phosphonic acid (VPA) to not only increase the number of acidic sites compared to many other polymer systems, but to also incorporate a super acid to help increase conductive pathways. 20%VZP co-VPA was synthesized via free radical polymerization to form a clear, flexible membrane with high proton conductivity. The film has been characterized using XRD, SAXS, FTIR, CPMAS NMR, TGA, DSC, PFGSE NMR and EIS. Characterization revealed an amorphous copolymer. Further tailoring and optimization of this system could yield a commercially viable fuel cell membrane.

Name: Katharine G. Dahm  
Degree Program: PhD  
Department: Environmental Science and Engineering  
Advisor: Jorg E. Drewes, Colette M. Van Straaten

Coalbed methane (CBM) is an unconventional gas source with large worldwide reserves. CBM wells are screened along coal seams, where water is produced to release pressure and allow methane to desorb from the coal surface (Orem, 2007). This practice has environmental impacts from disposal of co-produced, highly saline water. Industry treats co-produced water as a waste product. Water is commonly re-injected back into deeper aquifers for disposal. Lack of aquifer storage capacity directly limits gas production unless a solution for water treatment can be found. Regions in the US where CBM occurs in extractable quantities also are regions commonly experiencing water shortages. Utilizing produced water for irrigation, stream flow enhancement and drinking water augmentation is hindered by limited knowledge of water quality and variability. CBM produced water has total dissolved solid concentrations ranging from 1,500 to more than 30,000 mg/L (Benko and Drewes, 2008). In addition to dissolved inorganic constituents, naturally-occurring organic compounds are also present. High pressure membranes have the potential to desalinate produced water to standards required for beneficial use. Little, however, is known about the characteristics of the naturally occurring organic matter and impacts on membrane fouling.

Characteristics of organic matter present in produced water derive from sources within the system. Produced water samples, brackish groundwater, and deep-sea ocean water were evaluated to determine dominant chemical signatures. The carbon content in coal suggests dominant characteristics of organic matter in CBM produced water are derived from coal-water interactions. Coal samples were utilized in microcosm experiments to determine interaction chemistry of organic matter leaching off coal surfaces. Complexation of metals and organic matter dictate the size, active concentration, and dominate chemical identity of dissolved
organic matter. Complexation with ions, particularly heavy metals, determines the range of organic matter leaching off the coal surface as well as the in-situ organic and inorganic constituent distribution. Experimentation to determine the range of organic matter characteristics, type, size and concentration from different sources support evidence from microcosm experiments that a majority of naturally occurring organic matter originates from coal water interactions. Coal type organic matter characteristics and effects of metal complexation help to predict the potential impacts of coal derived organic matter on membrane fouling.


Solid-oxide fuel cells (SOFCs) offer great potential for efficiently converting biogas fuel streams into electricity across a wide range of power levels (kW to MW). Biogas produced through anaerobic digestion processes at waste-water treatment plants (WWTP) are flared at a rate of approximately 140 Mm$^3$ per day worldwide and generally consist of 65% methane and 35% carbon dioxide, after removal of trace contaminants. While biogas presents a significantly underutilized energy resource, this lower-quality fuel has high potential for carbon-deposit formation within the fuel cell, causing cell deactivation and failure. This necessitates use of a fuel reformer upstream of the fuel cell. By applying theoretical and experimental techniques, this study is focused on:

- Integrating an upstream fuel reformer into a SOFC system fueled by WWTP-derived biogas;
- Defining reforming strategies and operating windows for deposit-free SOFC operation; and
- Quantifying the electrochemical performance of SOFCs fueled by the biogas-reformate stream.

Many previous biogas-reforming strategies involve air addition; while this is a fairly simple and effective solution, system efficiency is reduced. This study explores the variation in reformed gas composition and cell performance by adding pure oxygen, carbon dioxide, and steam to the biogas stream prior to reforming. To explore these different strategies, two modeling techniques have been utilized. To determine equilibrium compositions and heat balances, chemical equilibrium modeling has been employed. A more-fundamental kinetic model has also been created using CANTERA software. This model includes the effects of porous-media transport, heterogeneous chemical kinetics, and energy balances within the reformer structure to predict gas composition and temperature throughout the catalyst foam.
These theoretical results are experimentally validated using the reforming experiment shown in Figure 1. In the experiment, a biogas mixture is simulated and mixed with the oxidant of interest before being fed to a quartz reactor containing a rhodium-based catalyst placed upon a rugged strontium-hexaaluminate support. The biogas-reformate composition is measured using a gas chromatograph. The reformate stream is also directed to an SOFC electrochemical test stand, and the cell is measure for performance as a function of the biogas-reforming approach. Results were used to quantify reforming strategy and cell-performance tradeoffs and to provide guidance on SOFC system design for use on biogas fuel streams.

Figure 1: Biogas reforming experiment; a) process flow diagram; and b) photograph.
New Route to Sulfonic Acid Functional Polymers

Name: Nathaniel T. Rebeck
Degree Program: MS, PhD
Department: Chemistry
Advisor: Daniel M. Knauss

A new route to sulfonic acid functional polymers has been developed, where a protected sulfonic acid moiety is used to carry out a controlled and directed sulfonation of poly(aryl ethers). These polymers have a variety of applications, however, the main focus of this research is to produce ion-conducting membranes and study this ion conduction at a fundamental level. By employing a protected sulfonic acid functionality, the acid will be generated in a controlled manner after polymerization to produce functional polymers without interfering with the polymerization. Using this process the properties of the polymer membrane can be adjusted by varying the position of the acid and the backbone linkages of the polymer. Studying these changes can give some insight into ion conduction in these materials.

In order to produce these new materials, a novel monomer was developed utilizing a sulfonamide moiety. This moiety has been used extensively as a protecting group for sulfonic acids and amines. It has also been shown to activate aryl halides for nucleophilic aromatic substitution but has never been used for polymerization. In utilizing this group to produce the desired materials, this research has shown the sulfonamide is a new activating group for nucleophilic aromatic substitution polymerization. This monomer produces high molecular weight stable polymers.
This work focuses on the system identification and control of a tubular Solid-Oxide Fuel Cell (SOFC) stack. In order to enhance the system efficiency and to avoid possible damages to the cell stack such as excessive temperature, coking or fuel starvation, the SOFC stack must be controlled within specific operating conditions. The need to maintain signal constraints during operation, combined with the importance of unmeasured variables such as internal stack temperature or fuel utilization, indicate the need for control-oriented models that can be used for estimation and advanced model-based control methodologies. Because of these important operating limits, as well as the strong interaction between input variables, Model Predictive Control (MPC) is a natural choice for control implementation. However, to implement MPC, a control-oriented model is needed that captures the dominant input-output behavior.

In this work, we present a systematic approach to the development of a control-oriented dynamic modeling of the SOFC stack using a Linear Parameter Varying (LPV) model structure. Based on the model developed in the identification stage, we implement an LPV-based MPC controller that can appropriately respond to the demand load over a wide range of operating point changes in real-time and improve transient performance while keeping the input/output variables within desired constraints. The LPV-based MPC controller is then tested on a detailed complex high-order model of the SOFC stack to show the effectiveness and capabilities of the proposed scheme.
Microbial Diversity Associated with Single Cell Protein Produced from a Brewery Wastewater Pilot Plant

Name: Jackson Lee  
Degree Program: PhD  
Department: Environmental Science and Engineering  
Advisor: John Spear

**Background:** Brewery wastewater typically contains large untapped amounts of useful dissolved carbon measured as Biological Oxygen Demand (BOD) that can be utilized for protein production for fish feed in the form of Single Cell Protein (SCP). Protein is produced from the growth of bacteria as it consumes carbon and is harvested and dried into a fishmeal replacement. Here we present results of a 1-year biodiversity monitoring study of a brewery wastewater treatment pilot plant tuned to produce a dried bacterial Single Cell Protein (SCP) fishfeed replacement product. The plant consistently produced 55-60% (w/w) crude protein SCP at about 15 kg/day. The key to this consistency was the addition of micronutrients to the wastewater during aerobic growth, but the exact microbial response to this addition was not well understood.

**Materials and Methods:** An initial survey of the brewery wastewater operations was conducted over the year 2008 using Sanger sequencing of the 16S SSU rRNA gene with the 8F/1492R primer. Samples were taken from throughout the brewery treatment works and pilot plant to establish a time course. Next, A 454 FLX pyrosequencing run was also completed using normalized DNA from the same samples as above with the bacterial 27F/338R primers and sample barcoding. Pyrotags were processed and clustered into Operational Taxonomic Units (OTUs) by the MOTHUR bioinformatics package.

**Results:** Ribosomal Database Project classifications of Sanger data showed that while the order level diversity was relatively simple, the consortia varied considerably both in time and in location. Pyrotag data (55,000 sequences) was characterized by a high degree of singleton OTUs. No single sequence comprised more than 2% of all sequences and no two samples (in either time or space) contained more than 10% OTU similarity. Phylum-level pyrotag diversity of the pilot production tank revealed dominance by Bacteroidetes followed by
Firmicutes and β/γ-Proteobacteria. Fast UniFrac results show that SCP product and pilot plant environments sometimes clustered together, and that some temporal clustering also occurs. More significantly, Fast UniFrac results show that each segment of the treatment works was highly selective. In order to understand where variations in Fast UniFrac data exist, a taxonomic rank abundance plot was made which details distributions of sequences within various phylum. Results show that major contributors to community structure lie in Firmicutes and Beta-proteobacteria, but the majority of dominant organisms come from Bacteroidetes, particularly from genus *Prevotella*, a group of carbohydrate metabolizing anaerobes commonly associated with tooth decay.

**Conclusion:** These results indicated that the bulk of diversity in the pilot plant were low count species and that high turnover led to considerable shifts in diversity within several major phyla, particularly from phylum Bacteroidetes, though overall protein concentration of the system remained consistent for the production of SCP. These results indicate that minute changes in reactor conditions commonly seen in day-to-day operations at any treatment plant can cause wide fluctuations in reactor diversity without impacting process stability.
Joint Denoising of a Signal Ensemble: the Power of Veto

Name: Alejandro Weinstein
Degree Program: PhD
Department: Engineering– Electrical
Advisor: Kevin Moore, Michael Wakin

This work presents a technique to denoise a signal ensemble by exploiting sparsity both at the inter and intra-signal level. The problem of signal denoising using thresholding estimators has received a lot of attention in the literature, starting in the 1990s when Donoho and Johnstone introduced the concept of wavelet shrinkage. In this approach, the signal is represented in a basis where it is sparse, and each noisy coefficient is thresholded by a parameter that depends on the noise level. We are extending this concept to a set of signals, under the assumption that the signals have a common support. Our approach is based on a vetoing mechanism, where in addition to thresholding, the inter-signal information is used to "save" a coefficient that otherwise would be "killed". Our method achieves a smaller risk than the independent denoising, and we quantify the expected value of this improvement. The results show a consistent improvement over the independent denoising, achieving results close to the ones produced by an oracle. We validate the technique using both synthetic and real world signals.
Quantum Many-body Tunneling of Bose-Einstein Condensates

Name: Joseph Glick
Degree Program: MS
Department: Physics (Applied Physics)
Advisor: Lincoln Carr

Consider the tunneling of a many-body wavefunction through a potential barrier. Specifically we examine quantum many-body tunneling of ultracold bosons in one dimensional optical lattice potentials. Such systems are described by the Bose-Hubbard model, and serve as an ideal testbed for the observation of quantum phenomena on macroscopic length scales.

Bright solitons, self-sustaining nonlinear waves, are confined by a thin potential barrier. By decreasing the size of the barrier or by tuning the nonlinearity, we find that the bound states can be transformed into quasi-bound ones as the soliton tunnels collectively out of confinement.

The lowly entangled 1D many-body problem can be numerically solved via time-evolving block decimation: a time-adaptive density matrix renormalization group routine. As a sanity check the results can be compared to mean-field theory predictions obtained from numerical analysis of the Nonlinear Schrodinger equation.

The goal behind this effort is to explore the previously intractable physics in regimes where the mean-field theory fails, and to provide a stringent test on the validity of quantum mechanics for complex entangled systems.
Heat treatment simulations provide a new capability to understand and predict complicated responses, where thermal, mechanical, and microstructural effects are coupled. Simulations using DANTE® compared the response of carburized and non-carburized 4120, 4320, and 8620 to oil and high intensity quenching. High intensity quenching involves high heat transfer rates and has the potential to reduce alloy content and carburization level compared to hot oil quenching. The simulations utilized a simple rod shape in order to minimize part geometry effects. The development of the microstructure, residual stress, and distortion are compared to understand the differences between high intensity quenching and oil quenching. The simulations predicted compressive residual hoop stresses at the surface for all high intensity quench conditions. In contrast, oil quenching produced compressive residual hoop stresses at the surface in the carburized condition and tensile residual hoop stresses in the non-carburized condition.
Within the past decade, NASA has been developing high temperature shape memory alloys (HTSMAs) for use as simple, robust, and lightweight solid-state actuators. Shape memory alloys (SMAs) as actuators are considered nonconventional and advanced actuation devices and are capable of providing a power to weight ratio greater than that of DC motors, pneumatic systems, and comparable to that of hydraulic systems, in a much more compact and simplified geometry. Alloys of Ni and Ti in equal amounts are the commercially prevalent SMAs, but are limited to uses near room temperature. Increasing the transformation temperature of traditional SMAs would allow for their use in various industries including aerospace, automotive, and down hole energy exploration, to name a few. Alloying additions of Pd, Pt, Au, Hf and Zr all increase the transformation temperatures of Ni-Ti alloys and at least potentially allow for their use in higher temperature applications. Pt is currently one of the most promising ternary additions for stable and predictable SMAs for use at high temperatures, but little is understood about the effects of Pt on the microstructure and mechanical properties of Ni-Ti alloys. The current research explores the link between alloy microstructures and the mechanical properties of several Ni-Ti-Pt alloys and the subsequent effects these relationships have on the overall performance of Ni-Ti-Pt HTSMAs as solid state actuators.
The Microstructural Response of 1045 and 4145 Steel to Induction Hardening

Name: Andrew Nissan
Degree Program: PhD
Department: Metallurgical and Materials Engineering
Advisor: Kip O. Findley

Induction hardening is a unique surface hardening technique that is used to increase wear and fatigue performance. Induction hardening allows for microstructural and residual stress characteristics that are not achievable by traditional furnace heating and quenching methods. Characterization of the resulting microstructure and hardness profile are of great importance in understanding the ideal case (hardened surface region)/core (unhardened subsurface region) ratio for optimal fatigue performance in service. In this study both 1045 and 4145 steel were induction hardened and characterized. To understand the effect of induction hardening on the microstructure and fatigue properties, two starting microstructures were selected for both alloys, normalized (softer more ductile microstructure) and oil quenched and tempered (harder less ductile microstructure) for the 1045 and as-hot rolled and oil quenched and tempered for the 4145. Each of these starting conditions were induction hardened to two depths (a low case depth and a high case depth) for a total of eight conditions. The initial and resulting microstructure was characterized by optical microscopy, scanning electron microscopy, x-ray diffraction, and microhardness traverses. A fatigue model based on the microstructure, geometric, and loading correction factors is proposed to determine the susceptible regions of the part due to fatigue. Some fatigue tests have been carried out to verify the validity of the model, and additional fatigue tests are planned to continually refine the model.
Hydrogen Peroxide Dynamics in an Agricultural Headwater Stream: Evidence for Significant Biological Production

Name: Taylor C. Dixon
Degree Program: MS
Department: Chemistry and Geochemistry (Hydrology)
Advisor: Bettina Voelker

Hydrogen peroxide (H$_2$O$_2$) is known to play key roles in aquatic systems, including metal redox cycling and degradation of organic matter into bioavailable forms. Detailed knowledge of the cycling of H$_2$O$_2$ in natural waters thus fosters the understanding of important aquatic biogeochemical processes. Although biological production of H$_2$O$_2$ has been observed in culture studies, the significance of this process to the H$_2$O$_2$ budget in freshwater systems remains unknown. In this study, isotopically-labeled H$_2$O$_2$ (H$_2^{18}$O$_2$) was added to novel in-stream mesocosm systems exposed to light and dark periods. By measuring total H$_2$O$_2$ and H$_2^{18}$O$_2$ in tandem, we inferred absolute rates of H$_2$O$_2$ production and decay, which were occurring simultaneously. The results indicate rates of H$_2$O$_2$ production up to several-fold the photo-production rates observed in filtered water samples, and suggest biological production as the dominant control on the H$_2$O$_2$ budget in the agricultural headwater stream studied. The potential implications of this work include enhanced understanding of freshwater metal and organic matter bioavailability, and natural attenuation of aquatic contaminants.
Part of the legacy of Uranium mining and milling includes the contamination of groundwater beneath and down-gradient from mill sites. Previously, techniques such as bioremediation have been used to attempt to address the plumes of Uranium contamination. Bioremediation of Uranium functions by pumping an electron donor into the subsurface to allow bacteria to generate energy through reduction of Uranium, Iron, and Sulfate. In the process, the Uranium is reduced to an insoluble form and thus mitigates the contamination in the water. However, current practice relies only on sampling at lengthy intervals and minimal adaption to address contaminant plumes. The REAL TIME project is working on detecting current subsurface contamination levels, redox activity, and remediation effectiveness in near real-time. This project, under the SmartGeo IGERT, is the combined effort of an interdisciplinary team with the ultimate aim of intelligently adapting the injection of electron donors into the subsurface using improved sensing and fusion of geophysical and chemical data, transmitted through a Wireless Sensor Network (WSN).

To date, the research has focused on combining physical and analytical methods to develop the ability to sense Uranium on a field sensor in near real time. The difficulty in this problem arises from the low concentrations of Uranium that need to be detected compared with other existing applications. The exploration of wireless sensor network integration with existing Uranium Sensors has been the primary focus of my work. Future plans include deploying a system at the Old Rifle, Colorado site to combine the Uranium Sensing with Geophysical methods to develop a better understanding of the bioremediation at the site. After deployment, investigation into the optimization of the injection of electron donor into the subsurface will occur, with the aim to develop a nearly autonomous system for the remediation of the Uranium.
The first requirement for any intelligent household energy management system is to be able to accurately measure energy usage in the home. Measuring energy usage is not difficult; however we must decide what to measure. Whole-home energy measurement is cheap and easy to setup because only one sensor is placed where the home connects to the power grid. The collected data can provide useful information for large appliances. However, the only way to monitor the energy usage of smaller devices is to install an energy meter on every device of interest. This creates a very detailed picture of household energy consumption, but requires a lot of additional hardware--one meter per device in the home. Here we explore an alternative, more practical, approach to monitor household energy usage including small devices. Our approach uses circuit-level power measurements and a new method to separate aggregate data into device-level estimates. Our initial evaluation resulted in an average error less than 5.35% for three devices with good response to changing device state. We therefore believe that this approach, coupled with a device-level control system, would create an ideal architecture for the next generation of household energy management systems.
Technique for Large-Scale EBSD Mapping of Polycrystalline Silicon

Name: Harvey L. Guthrey IV  
Degree Program: PhD  
Department: Metallurgical and Materials Engineering  
Advisor: Brian P. Gorman

The use of the electron backscattered diffraction (EBSD) technique to create maps of polycrystalline materials is generally limited to areas less than a square millimeter. In order to map larger areas, steps must be taken to address issues such as specimen preparation of large surface areas and orientation of these large specimens so they can be mounted appropriately in the microscope. Issues related to scanning areas larger than the SEM field of view and incorporating the results of these individual scans into a final map are also still challenges. In this work we present the procedure and results for EBSD mapping of a polycrystalline silicon wafer with an area of 156 X 156 mm$^2$. Techniques for field stitching, choosing pixel densities, and potential hardware modifications for EBSD mapping of large samples will be discussed.
Ionic hybrid nanostructures for energy conversion

Name: Archana Subramaniyan  Coauthors: Jianhua Tong, Daniel Clark
Degree Program: Masters
Department: Metallurgical and Materials Engineering
Advisor: Nigel Sammes, Ryan O’Hayre

Content withheld at authors’ request.
Constructing Rigorous MANET Simulation Scenarios with Realistic Mobility

Name: Aarti Munjal
Degree Program: PhD
Department: Mathematical and Computer Sciences
Advisor: Tracy Camp

One of the reasons that the MANET research community doesn’t have a standard routing protocol is because the protocols are not tested rigorously. Thus, it is important that the researchers choose an appropriate scenario to study the performance of a Mobile Ad hoc NETwork (MANET) via simulation. For example, routing is not properly evaluated when the shortest path between each pair of nodes in the simulation scenario is two or less. Various standards may be required to construct a credible MANET simulation scenario. In this work, we concentrate upon three standards for evaluating MANET routing protocols. Metrics involved in these standards are: average shortest-path hop count, average network partitioning, and average neighbor count.

Two standards, ensuring that the long routing paths are used to evaluate a generic routing protocol, have already been proposed in [1]. Quoting from [1]:

- **Standard 1**: To rigorously evaluate generic MANET routing protocols, the average shortest-path hop count should be large.
- **Standard 2**: To rigorously evaluate generic MANET routing protocols, the amount of network partitioning should be small.

In this work, we propose a third standard as follows:

- **Standard 3**: To rigorously evaluate generic MANET routing protocols, the average neighbor count should be large.

The main contribution of this work is to provide researchers with models that allow them to easily construct rigorous MANET simulation scenarios. The input to our models is the desired values for the three metrics mentioned; our models then output parameters for a simulation scenario that approximately meet the
researcher’s target values for the metrics. Our models were designed using a recently published mobility model that was constructed by extracting the statistical features of real human movement.

Our models enable researchers to test MANET routing protocols in a more realistic manner, thereby improving the credibility of their MANET simulation studies.

Mineralogy and its contribution to anisotropy and kerogen stiffness variations with maturity in the Bakken Shales

Name: Kene Mba
Degree Program: MS
Department: Petroleum Engineering
Advisor: Manika Prasad

The understanding of the controls on anisotropy and stiffness of the soft components (kerogens and clays) of organic-rich shales is important in developing methods for indirect and in-situ detection of maturity. Mineralogy of eleven Bakken shale samples with varying thermal maturities was studied to determine the contribution of mineralogy to anisotropy and kerogen stiffness variations between the shales. It was found that anisotropy increased with increasing clay content and that kerogen stiffness increased with maturity. Increasing clay content allows for increased micro-cracking during hydrocarbon expulsion, and so increased anisotropy. This clay-related anisotropy is independent of depth. Rock physics models aimed at the indirect prediction of maturity in organic-rich shales need to account for clay-related anisotropy and kerogen stiffness changes for better accuracy in impedance modeling.

Figure showing the averaging range soft components clay and kerogen (insoluble organic matter)
The Transformation of the U.S.-ROK Alliance: Balancing American Strategic Flexibility and South Korean Modernization

Name: Anthony F. Cerella  
Degree Program: MS  
Department: Liberal Arts and International Studies (MIPER)  
Advisor: Elizabeth Davis

Even though the bilateral security alliance between South Korea and the United States is a product of Cold War it remains strategically significant for Korean and Northeast Asian stability. The alliance is currently changing as both the United States and South Korea are modifying their military strategies and structures. The United States is currently transforming its defense structure centering on the idea of strategic flexibility. Strategic flexibility involves reexamining and reallocating global force structures to best combat a host of non-traditional threats. American transformation is changing the mission and scope of United States Forces Korea (USFK); considered the linchpin of the U.S.-ROK (Republic of Korea) alliance. Concurrently South Korea is assuming more responsibility for its defense and is instituting a detailed defense modernization plan known as the Defense Reform Plan 2020 (DRP). The simultaneous implementation of both plans will influence regional stability and test the long-term viability of the U.S.-ROK alliance. Simultaneous transformation will alter the alliance however, neither transformation plan calls for the elimination of the alliance. Joint synchronization of American and South Korean transformation plans; continued coordination and communication are the best policies to maintain the alliance. In sum this long-standing Cold War alliance remains valuable for the United States and Northeast Asia as it continues to promote regional security and stability.
Polymer Modification of Nanoparticles for Controlled Morphology of Nanoparticle/Polymer Films

Name: Melissa Kern  
Degree Program: PhD  
Department: Chemistry  
Advisor: Stephen Boyes

Thin film hybrid photovoltaics, which include organic donor and inorganic acceptor components, are attractive due to higher adsorption coefficients, more desirable mechanical properties, and less expensive processing. Despite these advantages, hybrid thin films have shown limited efficiency due to poor charge separation and extensive charge recombination. While bulk heterojunction devices improve charge separation, random pathways for charge transport are interrupted resulting in losses due to charge recombination. Therefore, control of film morphology at the nanoscale is essential for further improvements in device efficiency. The present work seeks to yield well-defined architectures by selectively incorporating nanoparticles into phase segregated polymer films of poly(3-hexylthiophene) (P3HT) and poly(styrene) (PS). Reversible addition fragmentation chain transfer (RAFT) polymerization provides well defined architectures with a trithiocarbonate end group that allows for facile attachment to nanoparticle surfaces. A novel P3HT macro-RAFT agent was synthesized to provide (1) a P3HT homopolymer and (2) a P3HT-b-PS copolymer that can be readily attached to the surface of gold nanoparticles through a thiol end group. Nanoparticles modified with the P3HT homopolymer would be incorporated exclusively into the P3HT domain of the polymer film, while PS homopolymer modified nanoparticles would incorporate into the PS domain. Furthermore, it is predicted that nanoparticles modified with a P3HT-b-PS copolymer would assemble at the interface between the domains in the thin film. Therefore, several different ordered film architectures can be obtained via polymer surface modification of nanoparticles prior to incorporation into phase segregated polymer films.
How to Build a Tricorder: Developing a Quantitative Habitability Prediction Tool for Planetary Exploration

Name: Kennda Lynch
Degree Program: PhD
Department: Environmental Science and Engineering
Advisor: John Spear, Tori Hoehler (NASA Ames Research Center)

Habitability of planetary environments is considered a principal theme in astrobiology. It addresses the fundamental question that is prevalent in the public mind: “is there life elsewhere in the universe?” As such over the past decade, planetary exploration has centered on a “follow the water” strategy in the search for evidence of extinct or extant extraterrestrial life. This approach has afforded a strong planetary exploration program, has focused astrobiological efforts for Mars and other solar system bodies and has produced a collection of appealing targets for future missions. However, merely following the water does not necessarily provide the full picture of habitability. The presence or absence of water and other constituents considered critical for life is simply a binary indicator of habitability that allows for delineation between habitable and non-habitable environments but results in an overabundance of “target environments”. Given the current mission constraints, it is unlikely that all “habitable” targets will be investigated with the scrutiny required to definitively determine evidence of life; this is especially true for in situ investigations on the planetary surface. Therefore, a more discriminating methodology is needed to optimize selection of target habitable environments.

It has been well described in microbial ecology that the distribution and success of microorganisms is governed by the availability of useful chemical energy and this energy can be quantified. From an astrobiological perspective, the extremes of energy availability have been studied in a fair amount of detail and applied to the binary model of habitability in the same manner as water and carbon. This goal of this research project is to evolve beyond this binary model and begin to develop a quantitative habitability metric that accounts not only for the relationship between energy requirements and energy availability but also for the environmental effects on both properties. The result being a habitability metric that addresses how habitable a
given environment is relative to its neighboring environment. This will allow future missions to conduct optimized searches & selection of the best target environments for further *in situ* analysis or for sample collection and return.
TestbedProfiler v2: An Improved Validation Tool for Wireless Sensor Network Testbed Deployment

Name: Josh Thomas  
Degree Program: MS  
Department: Mathematical and Computer Sciences  
Advisor: Qi Han

A key aspect of deploying a wireless sensor network (WSN) is understanding the degree of connectivity between the individual nodes that comprise the network. Towards that end, we present the second incarnation of TestbedProfiler, an application suite designed to aide the installation and improvement of WSN testbeds by revealing the characteristics of their underlying connections. Such knowledge allows node placement to be optimized to best fit the needs of a specific application. Originally developed with the capacity to evaluate network connectivity and performance based on transmission power level and packet size, the new TestbedProfiler can also measure the impact of specific radio channels and affords a much greater degree of control over its operation. Additionally, automated analysis of the resulting data now includes expected transmission count (ETX) and easily generated graphs that allow the connectivity of the network as a whole or of a single node to be visualized at a glance. The TestbedProfiler suite will be made freely available to other researchers and will hopefully lead to improved testbed deployments and better real-life WSN applications.
Solution Deposition of Amorphous IZO Films by Ultrasonic Spray

Name: Robert Pasquarelli  
Degree Program: PhD  
Department: Metallurgical and Materials Engineering  
Advisor: Ryan O’Hayre

Transparent conducting oxide (TCO) materials play a critical role in many current and emerging opto-electronic devices due to their unique combination of electronic conductivity and transparency in the visible region of the spectrum. This study examines the use of atmospheric-pressure solution processing as an alternative to conventional vacuum-based sputtering for the deposition of a recent archetype TCO material, amorphous indium zinc oxide (a-IZO). Solution processing is attractive due to its ease of fabrication, scalability, and potential to lower device manufacturing costs. Sputtered IZO shows the highest conductivity in the indium-rich region (~70 at%In) where the films are amorphous. However, current TCOs deposited by solution routes have only focused on crystalline, zinc-rich films (3-5 at% In). In nearly all these cases, acetate precursors are used.

Here we report on a-IZO films prepared by ultrasonic spray deposition from solutions of a novel indium-zinc formate (IZF) precursor. Films were sprayed between 100-210°C from an IZF-HNO₃-methanol solution and annealed under Ar-4%H₂. Thin films (<200nm) were produced with good optical transmittance (>80%) and conductivities of ~50 S/cm. Electronic carrier concentrations of the films were consistent with sputtered IZO (~10²⁰/cm³). However, the Hall mobility (~1cm²/Vs) is ~ 10–30X lower than sputtered IZO. Electron microscopy suggests the low mobility was due to porosity and film layering. Sputtered IZO is the most conductive in the amorphous region. X-ray diffraction of the sprayed IZO films showed that the amorphous state was successfully obtained after annealing at 300°C but that some phase separation of In₂O₃ occurred at 400°C. New precursors are being developed with the aim of both improving the electrical transport properties and reducing the thermal processing temperature.
Horizontal drains have been used since the 1930s to increase the stability of slopes by lowering the groundwater table. Since their inception many improvements have been made to the installation method and drain materials, including the development of horizontal wick drains. This new technique has proven effective at stabilizing slopes of predominantly silt and clay soils, while being less expensive and faster to install than traditional PVC pipe drains. Yet the adoption of this horizontal drain technique has been slow, in part due to uncertainty about the degree of clogging over long periods of time and when the drains may need to be replaced. To address these concerns, the reduction in flow rate compared to new drains was measured for exhumed wick drains that had been in the ground between one and 11 years. These measurements required the development of an apparatus to measure the flow rate through drain samples under constant head conditions. The results suggest that within the range of soil conditions in which horizontal wick drains are likely to be used, drain failure due to clogging is not expected. Visual examinations suggest that these drains are not as prone as pipe drains to iron or calcium precipitant buildup. While soil particle buildup does occur, the non-woven filter fabric provides numerous potential flow paths allowing sufficient water to pass even when much of the filter is clogged. The degree of clogging that a drain experiences is affected by the properties of the surrounding soil. Drains in soils made up of 85 percent or greater silt and clay exhibited a reduction in flow rate of up to 85 percent, while those in soils with 60 percent or less silt and clay displayed a reduction of no more than 42 percent. Despite these levels of clogging, horizontal wick drains are able to transport at least two times more water than the soil will introduce, even under the most demanding scenario expected. The critical reduction in flow rate necessary to cause drain failure is greater than 99 percent in the majority of anticipated scenarios.
Another outcome of this study is a chart used to select the proper drain spacing based on soil hydraulic conductivity and required drain length, in order to prevent exceeding the flow rate capacity of a drain.
Microbial and Substrate Characterization of Four BLM Biochemical Reactors in the Coeur D’Alene Idaho Area

Name: Roberta Martínez Hernández
Degree Program: MS
Department: Environmental Science and Engineering
Advisor: Linda Figueroa

The Bureau of Land Management (BLM) constructed four passive biochemical reactor systems (BCRs) to treat mining influenced water (MIW) in the Bunker Hill Superfund area near Coeur D’Alene, Idaho between 2002 and 2003. Initially, the BCRs operated very effectively. However, in the past couple of years, the zinc removal effectiveness of the four BCRs has declined.

These BCRs rely heavily on the presence of sulfate reducing bacteria (SRB), which produce hydrogen sulfide that precipitates dissolved metals out of solution. In order to insure long-term sustainability of passive treatment systems sulfate reduction levels must be sustained.

The central objective of this study was to characterize the microbial communities and substrate present within the BCRs and to use these factors to propose strategies to promote sustained sulfate reduction levels. Microbial communities were characterized by quantifying total bacteria and sulfate reducing species. Substrate was characterized by quantifying the percent organic, acid soluble organic, acid insoluble organic, and bioavailable material within the BCR.

The results suggest the depletion of bioavailable organic substrates is the primary cause of the decline in metals removal and not the microbial community structure. The ability to assess the amount of bioavailable organic substrate and microbial community is important to the understanding of the sulfate reducing capacity of the BLM BCRs and developing strategies to facilitate performance enhancement. The characterization of organic substrate and microbial community structure are also important to improving design of future passive treatment systems for mining influenced waters.
Study of Microalloy Precipitation in Hot Charged Slabs

Name: Myra S. Dyer
Degree Program: MS
Department: Metallurgical and Materials Engineering
Advisor: John G. Speer

As the demand for high strength and toughness of steel increases, the alloy design for HSLA grades is constantly being modified and tailored to available processing configurations. The effects of microalloy precipitation and (tunnel furnace) dissolution during Compact Strip Production (CSP) are explored relative to position within the slab (i.e. thermal profile of the slab), and alloy content. Niobium solute and precipitation fractions are quantified using electrochemical extraction and inductively coupled plasma atomic emission spectrometry (ICP-AES) techniques. The results are relevant in the content of cost effective alloying and increasing alloying efficiency.
Solution Processed NiO Modified Anodes in Bulk Heterojunction Organic Solar Cells

Name: K. Xerxes Steirer  
Degree Program: PhD  
Department: Applied Physics  
Advisors: Reuben T. Collins, David S. Ginley

Electrode surface modification is often used to optimize carrier selectivity and power conversion efficiency in organic photovoltaic devices. Presented are results from solution processed NiO thin films used as hole transport layers (HTL) in organic solar cells. We show how surface treatments of these films allow for modification of the as deposited electrode work function. NiO films on indium tin oxide (ITO) are then characterized via AFM and display rms roughness of 2.5 nm similar to that of ITO. The performance of NiO thin films are compared to a prototypical HTL, poly(3,4-ethelyne-dioxythiophene):poly(styrene-sulphonate) (PEDOT:PSS) in bulk heterojunction (BHJ) organic solar cells. Thin films of poly(3-hexylthiophene) (P3HT) on top of NiO or PEDOT:PSS are characterized with UV-vis absorption and show morphological differences depending upon the HTL. In devices, solution processed NiO modified anodes result in lowered series resistance and improved fill factors compared to similar devices using PEDOT:PSS. Photoconversion efficiency of P3HT:(1-(3-methoxycarbonyl) propyl-1-phenyl[6,6]C61 BHJ devices with the NiO layer reaches 4%. This efficiency is comparable to simultaneously prepared devices utilizing PEDOT:PSS for hole collection. Internal photoconversion efficiency plots of BHJ devices utilizing solution processed NiO HTLs exhibit lower efficiencies for wavelengths shorter than 580 nm relative to PEDOT:PSS based devices. The lower internal conversion efficiency is likely offset by the improved series resistance of the NiO HTL and thus gives a comparable overall efficiency.
Bose-Einstein condensates (BEC’s) in a honeycomb optical lattice are described by a nonlinear Dirac equation (NLDE) in the long wavelength, mean field limit [1]. The bipartite structure of the lattice appears as pseudospin in the multi-component BEC with states above and below the Dirac point playing the roles of particles and antiparticles. Although much work has been done on NLDE’s, the bulk of the literature deals with models with Poincare invariant nonlinearities. In contrast our equations break Poincare symmetry providing an opportunity to study phenomenological models in cosmology and particle physics where this symmetry is not manifest. We present the associated linear stability equations and apply them to the case of weak contact interactions to obtain the quasiparticle energies, states, and stabilities of vortex solutions of the mean field equations. We discuss future applications of our results to problems at the interface between condensed matter and particle physics. [1] L. H. Haddad and L. D. Carr, “The Nonlinear Dirac Equation in Bose-Einstein Condensates: Foundation and Symmetries,” Physica D: Nonlinear Phenomena, v. 238, p. 1413 (2009) .

http://arxiv.org/pdf/0803.3039v1
Predictive Bio-Computational Wear Modeling for Joint Replacements

Name: Jeffrey R. Armstrong
Degree Program: MS
Department: Engineering Systems – BioEngineering
Advisor: Anthony J. Petrella

Polyethylene wear has long been a topic of concern for the longevity of joint replacement systems as bearing failure is the leading cause for the need of revision surgery. Experimental simulations are costly and time consuming; therefore, a more efficient solution for predicting wear is computer simulation. Predictive computational modeling of the adhesive/abrasive wear mechanism has been in use for over a decade, but the accuracy of such models is still under debate \[1\text{–}7\]. Recent studies have shown that cross-path motion, as seen in joint replacements, results in elevated wear and shortens the life of the polyethylene bearing surface \[8\text{–}10\]. Modern computer simulations have attempted to address the effects of cross-path motion and range from simple to complex formulations \[9, 11\text{–}13\]. Current models are limited by their complexity, computational efficiency, joint-specificity, or motion-cycle path dependence.

In this study, an adaptive finite element (FE) model was used to implement a modified form of Archard’s Wear law \[1\] that accounts for the effects of cross-path motion and polymer chain realignment. The proposed model was validated to three separate experimental wear systems, each with three loading scenarios. As seen in Equation 1, the proposed Modified Archard’s law sums the effects of unidirectional and cross-path motion and also accounts for polymer chain realignment, referred to as ‘memory’. This Modified Archard’s law is simple and generally applicable to any wear system:

\[
\text{Wear Depth} = k_0 \sum_i p_i \cdot s_i + k^* \sum_i p_i \cdot s_i \cdot m_i \quad \text{Eqn. (1)}
\]

where ‘\(k_0\)’ and ‘\(k^*\)’ are experimentally derived wear coefficients for uni-directional and cross-path sliding, respectively. The variable ‘\(p\)’ refers to contact pressure and the variable ‘\(s\)’ is the magnitude of incremental
sliding distance. The variable ‘m’ incorporates memory and sliding trajectory effects; its full definition can be found in [14].

Validation of the proposed wear model was completed through comparisons to published experimental data for three wear systems. The first system was a pin-on-disk wear experiment by Dressler et al. [15]. They concluded that wear was elevated by changes in direction but that the elevated wear diminished with sliding in a consistent direction up to 5 millimeters. Application of previous models to this experimental system resulted in incorrect wear predictions. Application of the proposed Modified Archard’s law was able to predict the experimental wear volume results exactly.

Further validation was confirmed when the Modified Archard’s law was applied to FE models of a cervical disk replacement and a total knee replacement, as seen in Figure 1. The cervical disk model was made in accordance with the experimental setup by Bushelow et al. [16]. The total knee replacement model was made in accordance to the setup by McEwen et al. [10]. Experimental wear depth and volume results were compared to predictions from both the classical and Modified forms of Archard’s Wear law for each of the two experiments’ three distinct loading scenarios. Wear coefficients were scaled to a standard loading scenario for each system. In each of the two predicted scenarios of both experiments, the Modified Archard’s Wear law showed a better fit to the experimental data than the classical Archard’s Wear formulation.

![Figure 1](image_url)

**Figure 1** – (a) Cervical Disk Replacement hardware  
(b) FE model of a Total Knee Replacement system
Continuous Compaction Control (CCC) and Intelligent Compaction (IC) rollers promise large potential improvements for earthwork construction. CCC rollers provide a spatial measure of soil properties (e.g., stiffness) over the earthwork surface. CCC rollers can be used for quality control/quality assurance (QC/QA) to enable compaction based feedback control and to create as-built documentation. CCC rollers offer great promise for QC/QA by enabling 100% evaluation of an earthwork area during every roller pass, in contrast to current quantitative QC/QA which evaluates less than 1% of the earthwork after a few roller passes.

Experimental data has shown that vibratory roller compactors often exhibit rotational kinematics in addition to translation during operation. This rotation is not considered in the current generation of roller measurement values. A new roller/soil model that allows for rotational kinematics was developed. Using the model, the influence of sensor position on roller measurement values is examined. The influence of drum rotation is shown to be significant. Building upon these findings, a new technique is developed for computing roller measurement values while negating the influence of rotation. This new technique is shown to be directionally independent. The new measurement technique is compared verse the current measurement technique for common CCC roller tasks.
A Model for the Envelopes of Spin Waves in Magnetic Film Feedback Rings

Name: Justin Q. Anderson
Degree Program: MS
Department: MACS
Advisors: Lincoln D. Carr, Luis Tenorio

Experimental observation of spin wave envelopes (SWE) in magnetic thin films necessarily occurs in non-conservative systems. The generation of time-stable results is realized by approximating conservation through active feedback, or otherwise driving the system into equilibrium with its major linear loss mechanisms. A rich variety of SWE nonlinear dynamics have successfully been observed in “conservative” systems of this form, including chaos, soliton formation, and more recently, a chaotic modulation of solitary wave train envelopes.

The dynamics of these “conservative” systems have often been modeled by a 1D Ginzburg-Landau Equation (GLE) of the general form, 
\[-\partial_t \varphi = (D \partial_{xx} + N|\varphi|^2)\varphi,\]
where \(D\) and \(N\) are real parameters corresponding to the system’s inherit dispersion and nonlinearity, respectively, and \(\varphi\) is the SWE wavefunction. Extension to multiple dimensions is the trivial introduction of a Lapacian operator in place of the spatial derivative. The GLE is a fully conservative equation which has succeeded in modeling SWE solitons in these dissipative systems. However, the cubic GLE does not yield chaos and the severity of the nonlinear term, which is a function of the wavefunction normalization, exhibits time dependence in any dissipative system due to loss and gain.

A driven damped model is proposed to overcome the shortcomings of the traditional GLE and is studied numerically in the context of the chaotic modulation of solitary waves. The model is a cubic, quintic complex GLE (CGLE) with constant gain,
\[-\partial_t \varphi = (D \partial_{xx} + (N + iG)|\varphi|^2 - iL - (Q + iS)|\varphi|^4)\varphi,\]
where all constants, \(D, N, G, L, Q, S\), are real. This modification of the GLE introduces higher order nonlinearity and a gain/loss mechanism at linear, cubic, and quintic orders.
A preliminary investigation of the CGLE is reported and a qualitative agreement of simulations with experimental observation is demonstrated. A saturation of cubic nonlinearity, of the four-wave process, is suggested as the driving force behind the chaotic modulation of magnetic SWE solitary waves, and predictions of experimentally achievable chaotic domains are presented.

This work is supported by the U.S. National Science Foundation.
Afternoon Poster Session Abstracts
Analysis of Trace Organic Contaminants in Raw Wastewater at various sewershed scales by Liquid Chromatography-Tandem Mass Spectrometry

Name: Jennifer Teerlink
Degree Program: PhD
Department: Environmental Science and Engineering
Advisor: Jörg Drewes

The past decade has seen a vast increase in research related to the fate and occurrence of Trace Organic Contaminants (TOrc) in natural and engineered systems. TOrc include compounds found in personal care products, flame-retardants, detergents, pharmaceuticals, and plasticizers. Advances in analytical techniques have led to the quantification of these compounds to the low ng/L concentration range. Even at these low concentrations some compounds have shown carcinogenic or endocrine disrupting effects. Throughout the literature the occurrence of TOrc is being reported for raw sewage, wastewater effluent, surface water, groundwater, and drinking water. Because of the sheer number of compounds present it is important that research efforts are prioritized. Three possible approaches are to focus on compounds that are 1) used in greatest abundance, 2) most persistent, or 3) have known endocrine disrupting, other physiological effects.

Wastewater is the primary route of introduction for TOrc. Wastewater treatment can vary from advanced centralized facilities designed for large urban centers to decentralized septic systems serving a single family home. The literature to date suggests that in both types of treatment systems many compounds are effectively removed. However, other TOrc persist. It is imperative to understand the TOrc loading to various wastewater treatment facilities in order to design for maximum loading rates and understand loading rate to the ultimate receiving environment.

This study was designed to gain a better understanding of the variability in TOrc loading based on sewershed size. Three locations were selected: 80,000 person centralized wastewater treatment facility, medium decentralized clustered system serving 400 people, and a small 16 person septic system. Sampling at
each location consisted of hourly sampling for 26 hours. Samples were analyzed for 45 compounds with limit of quantification ranging from 2.5 to 250 ng/L using liquid chromatography with dual mass spectrometry and stable isotope dilution. This method has been verified for this complex matrix of raw wastewater in this study.

The greatest variability and highest individual loading rates were found in the smallest system. Greatest average loading rates were found in the large centralized system. For a select subset of compounds usage data and population were used to calculate if measured values were reasonable.
Reservoir characterization, modeling and simulation are a necessary part of any enhanced oil recovery program. Today there have been many advances in both static and dynamic reservoir modeling but as new levels of complexity are introduced, we also introduce the demand for more computing power and computation time. Optimizing the modeling process without sacrificing model integrity has the potential to save valuable resources and aid in overall efficiency.

Postle Field is a mature oil and gas field in Texas County, Oklahoma which produces from Pennsylvanian valley fill sandstones. EOR practices, in the form water flood and CO2 miscible flooding in the field have led to the need for reservoir modeling and simulation in order to increase recovery.

Incised valley fills are complex and it is often difficult to achieve realistic static models because of severe heterogeneity, issues with data resolution, upscaling and lack of computation time and power. This study focuses on optimizing the modeling process by exploring how models change as a function of input parameters, such as cell dimensions, inclusion of stratigraphically significant surfaces, facies modeling and geobody types, as well as incorporation of additional seismic and geo-statistical data.

A total of thirty two different model types were created each varying systematically in complexity. Thirty realizations of each model type were run yielding 960 total models. Pore-volumes were calculated for each model and averaged according to model type for comparison. Selected models were then simulated and compared using both the full field and individual well performance history matches.
Results of the static comparison show marked contrast between models using channel-form and bar-form geo-bodies. Models using bar-forms consistently reproduced reservoir volumes indicating that simpler models may be sufficient. A static volumetric match is not enough and models must be history matched to assess their dynamic performance. Dynamic results show that history matches are significantly improved with addition of data, particularly vertical proportion curves. Despite constant static matches, improvement in history matching results demonstrates the need for integration of multiple data sets at many scales to accurately represent geologically complex reservoirs. The results of this study help to define best practices for static modeling in valley fill systems; optimizing time, resources and increasing overall efficiency.
Rheology & Chemical Characterization of Alaska Heavy Oils

Name: Chenru (Victor) Zhang
Degree Program: PhD
Department: Chemical Engineering
Advisors: Andrew M. Herring, Matthew W. Liberatore

Introduction

Although the reserves of heavy oil on the North Slope of Alaska are enormous (an estimate of at least 10 billion barrels are in place), difficult technical and economic hurdles are involved in producing these oils. The Ugnu formation contains the most viscous, biodegraded oils and standard production methods will be ineffective. Numerous alternative techniques for heavy oil production have been proposed (cold production, steam injection, etc). The overall objective of the project at Colorado School of Mines is to advance the state-of-the-art of seismic monitoring, using chemical and physical characterization of core samples in combination with simulated production experiments, to optimize the recovery of heavy oils from Alaskan deposits. A preliminary study showed that we could correlate chemical information with rheological data. New data will be presented concerning the non Newtonian rheology and chemical characterization by various techniques on samples from the Ugnu formation.

Experimental

Microscope Characterization. In order to work out the settling properties of the sand in the oil, the diameter distribution of the sand need to be quantified. The optical microscope Olympus IX81 was employed to take pictures of the sand grains, which was already dispersed in the mineral oil in advance in order to simulate the real conditions in the test.

Rheology Testing. The rheological properties of the Ugnu Samples were measured at five different temperatures. The frequency range was 0.001 to 100 Hz at a fixed stain of 0.1, using an AR-G2 rheometer with
40 mm plate geometry at the operating gap of 1000 mm. To see how the Ugnu heavy oil changes its properties, a sequence of experiments on the heavy oil with different sand cuts were conducted.

**Molecular Beam Mass Spectrometry (MBMS).** Helium was used as the carrier gas with the flow rate of 150 ml/min. The temperature rises from 50 to 750 °C with the rate of 15 °C/min.

**Results and Discussion**

**Size Distribution of the Sand.** With the help of the software ImageJ, the perimeters P and the areas A of more than 2,500 particles were measured, and then the average diameter is determined to be 5.31 μm, with a standard derivation of 5.57 μm.

**Rheological Properties.** Figure 1 shows that the viscosity of the Ugnu sample as received decreases with temperature, which is not surprising. Furthermore, the viscosity and shear thinning degree of heavy oil changes with sand and water content. The dependence of rheology on sand content is strong, while that on water content is weak.

![Viscosities of the Crude Oil as Received](image)

Figure 1. The rheological behavior of the Ugnu heavy oil as received
MBMS result shows that there are three regions of reactivity during the pyrolysis. The initial volatility takes place at 100 to 150 °C; the maximum vapors show up at 200 to 300 °C; and the cracking appears at 550 to 700°C.
Electrochemical Behavior of Titanium and its Alloys in Simulated Body Fluid

Name: Rahul Bhola
Degree Program: PhD
Department: Metallurgical and Materials Engineering
Advisors: Brajendra Mishra, David L. Olson, Reed A. Ayers

The electrochemical behavior of beta titanium alloy, Ti-12Mo-6Zr-2Fe alloy has been characterized in phosphate buffer saline solution at the physiological temperature and the results have been compared with that of commercially pure titanium (grade 1-alpha) and Ti-6Al-4V (alpha & beta). The impedance data for the alloys was found to fit a two-time constant circuit model. The alloys are attacked by chloride ions from PBS solution, but eventually they are able to reconstruct the depleted oxide layer. In the passivation range, the alloys show a marked increase in the barrier resistance, confirmed from EIS results, but at further higher over-potentials, the barrier layer becomes defective, resulting in a decrease in the barrier layer resistance values. The corrosion potentials of the reverse scan curves for the alloys are anodic to the corrosion potentials of the forward scan curves, which signifies a high pitting corrosion resistance of these alloys.
As the interest in renewable energy increases, an effort to achieve an environmentally clean and efficient energy source is becoming more important. Hydrogen provides the highest mass based combustion energy of any fuel. Currently, there are three main hydrogen storage materials: metal hydrides, chemical storage, and carbon-based materials. All these materials have advantages and disadvantages. In addition to these materials, clathrate hydrates have been investigated as a hydrogen storage material. Initially, it was thought that hydrogen would not form hydrogen hydrates because of its small molecular structure, but recent experiments have shown this can be achieved.

There are several advantages and disadvantages of using clathrate hydrates as a hydrogen storage material. Firstly an advantage, the system is largely composed of water. Because of this, there are no harmful byproducts when the hydrogen is released. In addition, the hydrogen can be released by simply de-pressurizing the system (by turning a valve). Therefore, no chemical reaction is required. However, the disadvantage of using clathrate hydrates is that the stability condition for hydrogen hydrates is at very severe conditions: very high pressures and low temperatures. In addition, the storage capacity of hydrogen is low.
In order to alleviate the severe conditions, promoter molecules are used to shift the phase equilibrium boundary to lower pressures and higher temperature conditions. However, the addition of a promoter molecule reduces the possible storage capacity for hydrogen. For example, tetrahydrofuran is commonly used as a promoter molecule in the hydrogen hydrate system. Other molecules can be used as well.

The purpose of this experiment was to introduce a new synthesis method for using tetrahydrofuran as a promoter molecule to increase the hydrogen storage capacity of a hydrogen hydrate system. Results indicate the hydrogen and tetrahydrofuran molecules compete for cage occupancy within a certain composition range. It was concluded that up to 3.4 wt% hydrogen was stored using this method. Previously, it was believed that a hydrogen storage asymptotes to about 1.0 wt%.
Determining a Rheological Protocol for Measuring the Fluid Properties of Bio-oil

Name: Michael Nolte
Degree Program: MS
Department: Chemical Engineering
Advisor: Matthew Liberatore

Bio-oil, produced from the pyrolysis of biomass, is a renewable and carbon neutral fuel that is gaining more attention as a replacement for petroleum-based fuel oils. However, it currently has some drawbacks that are preventing it from becoming a more widely adopted fuel. Namely, bio-oil has a high water content (~15-30%) and high oxygen content (~44-60%), which reduce the heating value of the oil. Bio-oil is also acidic (pH of ~2-4), reactive when it is first produced, and it may become unstable and separate into two phases during storage. Current research is aimed towards upgrading and stabilizing bio-oils through catalysis, esterification, emulsification into diesel fuel, steam reforming, and/or the addition of solvents.

Knowing the viscosity of bio-oil and how it changes with time, temperature, or composition is important for purposes such as pumping, atomization, etc. Since bio-oils are relatively new field of study, there are currently no standards available that dictate a procedure for measuring the viscosity of a bio-oil sample. A review of the literature finds that some researchers use the ASTM D-445-88 standard for petroleum oils. Others use simple cup and bob viscometers at a few temperatures and/or shear rates. The goal of this research is to determine the proper protocol for rheological measurements of bio-oils and to possibly correlate the viscosity of the oil with its properties (including water content, pH, feedstock, or other physical property).
The vast majority of fossil assemblages from the Archean are highly biased toward filamentous and coccoid morphologies, and consist of silicified microbes that lived in mat communities and solute-rich waters. This apparent preferential preservation of microbes with certain morphologies and living strategies implies that entire ecosystems of organisms were intrinsically excluded from the fossil record, providing us with a skewed view of early life on Earth. In addition, interpretation of these fossils is extremely difficult and is based primarily on morphological comparisons to extant microbes. But working back from fossil forms to reconstruct a fossil organism’s life form is next to impossible as most taxonomically identifying features become obscured early in the silicification process, and what remains is easily erased through diagenetic alteration. The mechanisms that surround and dictate the process of silicification are very poorly constrained. Even more poorly understood are the mechanisms that control the preferential silicification of some organisms over others. This work is composed of collaborative and interdisciplinary research that integrates field and laboratory experiments to elucidate which biological characteristics are most important in the silicification and subsequent preservation of microbial cells today and throughout life’s history here on Earth.

The field component of this proposed work is centered in the Lower Geyser Basin of Yellowstone National Park. Four hot springs of similar chemistry and morphology lie aligned in the Lower Basin but Steep Cone Hot Spring (Steep) is the only one that is actively accumulating a silica deposit. Steep is an approximately 12 meter tall hot spring deposit composed of laminated, lithified microbial mat. Due to a rock fall, approximately ten vertical meters of fossil mat sequence is exposed, and unlike many relic hot spring deposits,
the fossil sequence at this site is capped by its modern, living microbial mat. The existence of living, half-lithified and lithified mats side-by-side provides an invaluable opportunity to examine the lithification process while minimizing the probability that they have experienced extreme diagenesis or changes in hot spring chemistry over time. In addition, we can directly compare the living and lithified mats to see what changes have occurred through the lithification process and diagnose which microbe(s) create the framework of the lithified mat.
Solid-oxide fuel cells (SOFC) have generated interest recently due to their ability to efficiently convert a broad range of hydrocarbon and biomass fuel sources into electricity. However, the propensity for carbon-deposit formation and subsequent catalyst deactivation limits the operating conditions under which SOFCs may operate. Developers are taking many different approaches to solving these problems. Numerous anode materials and architectures are being developed and tested, such as Ni-YSZ cermets, cermets with inert barrier layers, cermets with active catalyst layers, and nickel-free perovskite or copper anodes. With standard SOFC tests, however, it is difficult to discern specific information about an anode's gas transport and catalytic activity properties. These properties are central to an anode's ability to operate successfully on hydrocarbon or biomass fuels.

This study decouples anode chemistry processes from the electrochemistry processes present in the operation of an SOFC through the use of a unique experiment. In the Separated Anode Experiment (SAE), a single SOFC anode channel is simulated by sealing an anode between two ceramic manifolds into which flow channels have been machined. An illustration of the SAE is provided in Figure 1. Gases representative of SOFC fuel streams are fed into the "fuel channel", while gas mixtures representative of the products of electrochemistry (H₂O and CO₂) are fed into the "electrolyte channel". Gases from these two channels are then free to cross-diffuse...
through the porous anode and participate in internal-reforming reactions. Exhaust-gas compositions are measured with a mass spectrometer and are used to infer details regarding the anode's gas transport and internal reforming activity.

Interpretation of the experimental results is aided through the use of a computational model which incorporates channel gas flow, porous-media transport, and elementary heterogeneous chemical kinetics. The model can serve as a design tool for anode morphology optimization. In addition to advancing our fundamental knowledge of processes occurring within an anode structure, these tools also allow for performance comparisons to be made between the various anode materials and architectures being developed. Both flow channels are modeled using steady-state, plug-flow assumptions. Porous media transport is represented by the Dusty-Gas Model, which incorporates multicomponent gas diffusion, Knudsen diffusion, and pressure-driven Darcy flow. The DGM uses material properties which are quantified and input into the model.

Five different materials and structures are compared in this study on the basis of their gas transport and internal-reforming abilities. These materials are a CoorsTek, Inc. reaction-sintered Ni-YSZ, a traditional Ni-YSZ with anode functional layer (AFL), an inert YSZ barrier layer, a CoorsTek Ni-YSZ and barrier bi-layer anode, and a new-generation perovskite anode.
Characterizing the meso-scopic dynamic properties of soil is necessary for a multitude of civil engineering applications. Strain-dependent shear modulus, $G$, and damping ratio, $\xi$, are easily determined from meso- or element-level resonant column tests and established models based upon wave theory and continuum material dynamics. However, the damping ratio curve for a soil is a meso-scopic measurement that is based upon particle-level, dissipative interactions of the soil being tested. With this in mind, research is necessary to pinpoint the micro-scale factors responsible for variances in damping ratio between soil materials.

QEMSCAN technology has been pioneered to measure the average sphericity of sand samples with quantified particle size distribution curves. These particle-scale measurements have been used to help predict the damping characteristics of the samples tested and are compared to element-scale damping curves measured using the element-level resonant column tests. More clearly understanding the relationship between the micro-scale characteristics of a soil and the meso-scale measurements typically used in civil engineering applications may lead to predictive relationships based upon particle-level properties for the damping characteristics of a given soil.
Optimization of connections between feeders in an emerging distribution system

Name: Hilary E. Brown
Degree Program: MS
Department: Engineering
Advisor: Siddharth Suryanarayanan

The Energy Independence and Security Act of 2007 outlined the “Smart Grid” as the desired method of modernization for the US electric power system. Using results from an industry survey seeking a definition of a smart distribution system, characteristics of emerging distribution systems are applied to a distribution test system. An optimization problem called ‘the feeder addition problem’ is defined to determine the locations of new connections between feeders in a radial distribution system to improve the reliability of the islanded system. The constraints considered include the operating requirements, such as voltage levels and branch loading. This multi-objective optimization problem balancing cost and reliability is solved using a heuristic technique and the application of a multi-objective genetic algorithm. Both methods are applied to a common reliability test system and the optimization results are given.
Assessing DNAPL dissolution kinetics a bench-scale fracture network

Name: Kaneen E. Christensen  
Degree Program: PhD  
Department: Environmental Science and Engineering  
Advisor: John McCray, Charles Schaefer

Dense non-aqueous phase liquid (DNAPL) present in fractured bedrock settings introduces unique remediation challenges that are significantly different from porous media. This research is the first to explore the dissolution behavior of tetrachloroethylene (PCE) DNAPL in a bench-scale three-dimensional (3-D) sandstone fracture network during ambient groundwater conditions and compare these results to DNAPL dissolution during chemical oxidation. Prior to the chemical oxidation experiments, two types of aqueous-only dissolution experiments were performed. Effluent concentrations of aqueous phase PCE were monitored and interfacial area tracer tests were used to quantify DNAPL interfacial areas over the course of the ambient groundwater experiments and rates of the dissolution mass-transfer. All experimentally derived mass transfer rates will be evaluated against system properties to determine the primary factors controlling DNAPL dissolution in a fracture setting: interfacial area, aperture variability, dispersivity, DNAPL Saturation, Reynolds number and Péclet number.
Wind turbines have grown in size dramatically over the last three decades for many reasons, including advances in research and development and economies of scale. Large modern wind turbines push the envelope on safety factors related to fatigue and extreme loads compared to their smaller, older counterparts. Advanced feedforward and feedback control techniques can help to reduce these structural loads over a range of operating conditions. Of particular interest in industry is the mitigation of tower and blade root bending loads, which can be achieved via advanced control.

Two advanced controllers shown in Figure 1 designed to reduce wind turbine component loading have been developed. The advanced controllers attempt to damp tower fore-aft and blade root bending moments using tower fore-aft and blade flap tip signals in feedback to augment the commanded pitch angle of the baseline controllers.

Figure 2. Advanced controllers designed to reduce wind turbine component (tower and blade root bending) loading
The tower damping controller uses tower velocity feedback to augment the commanded pitch component of the baseline controller. The dominant tower motion is assumed to be characterized by the tower first fore-aft mode. The amount of tower damping is adjusted by changing the value of a tower feedback gain $G$. The tower and blade damping controller combines a blade flapwise bending moment reduction with a tower damping and is realized using full-state-feedback. The tower and blade damping controller, designed to damp tower first fore-aft moment and blade flapwise moments, uses velocity and displacement of tower-top first fore-aft mode, and the blades’ perturbed flap tip velocity and displacement as individual pitch command feedback to augment the commanded pitch component of the baseline controller. The authority of the tower and blade damping controller is adjusted by changing the value of “Feedback Gains”, which is a 3 by 8 matrix. The three baseline controllers considered in this study are a PI feedback only collective pitch controller, a combined feedback/feedforward collective pitch controller, and a combined feedback/feedforward individual pitch controller.

A full set of 279 realistic wind input files are used for the simulations. Simulation results in these turbulent wind fields demonstrate that adding fore-aft tower damping and blade damping to standard baseline controllers can give effective mitigation on the tower fore-aft and blade flapwise bending moment without reducing power production as shown in Figure 2. Compared to the baseline, the tower and blade damping controller reduces the tower base fore-aft bending moment by at least 13%, and the blade flapwise bending moment at root by at least 8%. Tower and blade damping plus a combined feedback/feedforward collective pitch controller (FFCP) reduces the tower side-to-side bending moment by a magnitude of almost 40%.
Figure 3. Simulation results comparisons with their corresponding baseline controllers
Locating abandoned coal mines to assess subsidence risk using self-potential and DC resistivity, Weld County, Colorado

Name: Karoline J. Bohlen
Degree Program: MS
Department: Geophysics
Advisors: André Revil, Mike Batzle

Historically, there has been heavy coal mining in Boulder and Weld Counties, Colorado. The majority of the coal was mined using the room and pillar method. With this method, working areas, or “rooms” are carved into the coal seams with “pillars” of coal left intact to support a roof structure during the mining. As the coal seam end is met, the mining equipment and personnel retreat towards the entrance, extracting coal from the pillars as they retreat. Over time, sinkholes can appear where these mining rooms were created and the unsupported roofs collapse.

Much of the old mining areas have been developed for residential and commercial use. Poor documentation of coal mine locations in the past and current safety concerns (see Figure 1) have lent urgency to assessing subsidence potential in these historical mining areas. A need for geophysical methods exists that can be used to determine areas where hazardous and economically damaging subsidence incidents could develop. With such tenuous subsurface areas, it was determined that any survey method(s) utilized for this assessment must be as non-intrusive as possible, due both to residential concerns and personnel safety.

We show here that by using a combination of the self-
potential (SP) and DC resistivity methods, we can identify existing and possibly potential subsidence locations in an area of abandoned coal mines. The data from a survey utilizing SP and DC resistivity presented results that agreed with existing maps and also indicated areas that require further investigation.
Hole Cleaning using “Conventional and Enhanced Sweep”

Name: Thanh Ngoc Nguyen
Degree Program: PhD
Department: Petroleum Engineering
Advisor: Yu Shu Wu

Content withheld at authors’ request.
Heap Leaching: A New Approach to Uranium Mining Waste Utilization

Name: Erik Hunter  
Degree Program: PhD  
Department: Mining Engineering  
Advisor: Mark Kuchta, Linda Figueroa

Uranium mining and milling in the Western United States has resulted in the accumulation of millions of tons of waste material that contain a significant amount of uranium and vanadium. Although current waste disposal techniques have been proven sound from an environmental standpoint, the high cost of disposal is a limiting factor in the overall number of sites that can be remediated. Environmental groups and citizens of Western states have put pressure on state and federal government agencies to clean up legacy uranium mine sites. This pressure has resulted in a significant amount of reclamation activity by government and private industry.

The purpose of this thesis project is to evaluate the use of oxidants in an alkaline heap leaching system designed to recover uranium and vanadium from mining waste. The goal of the proposed experiments is to prove that oxidants can be used to accelerate the rate of uranium recovery, and therefore improve the economics of alkaline heap leaching. The project will be focused on the Grants Ridge Armijo mining venture which is located in Grants, New Mexico. Grants Ridge is a joint venture between Uranium Energy Corporation (UEC) and Uran Limited. The site, which includes both private and federal land, is heavily disturbed by historic uranium mining activities. Waste dumps with significant uranium mineralization exist at the project site. Uran Ltd. will construct and operate the second commercial scale heap alkaline uranium heap leach in history.

This project will prove that heap leaching and reclamation of uranium waste dumps is an economic alternative to traditional onsite burial and reclamation. The specific tasks include:
Task 1: Bench scale alkaline leaching experiments will be performed on limestone uranium ore. The experiments will involve both agitated and column leaching. A variety of oxidants will be used and their performance will be evaluated.

Task 2: The experimental data will be evaluated and modeled according to established principles of thermodynamics and hydrometallurgy. A reagent and oxidizer scheme will be chosen for the pilot scale experiments based on the bench scale experimental results.

Task 3: Pilot scale column and/or heap leaching experiments will be performed using the most effective alkaline reagents and oxidizer combination.

As the application of alkaline heap leaching to uranium recovery is a new field, there is little data concerning the effect of oxidizers on leaching kinetics. This study will provide valuable data and conclusions that will advance the understanding of the role of oxidizers in alkaline heap leaching.
Fault Tolerant Linear Algebra: Recovering from Fail-Stop Failures without Checkpointing

Name: Teresa Davies
Degree Program: PhD
Department: Mathematical and Computer Sciences
Advisor: Zizhong Chen

As the number of processors used for a calculation increases, so does the probability that one or more will fail before the calculation is complete. There are a number of methods for recovering lost data in the event of a failure, so that the computation can proceed with a smaller loss of time than if it had to be restarted. However, all methods introduce some overhead, including for cases where no failure occurs.

One common technique is checkpointing, which involves writing a copy of the data into storage at some interval, depending on the type of computation and the probability of a failure. It is a well developed technique, and is effective for a wide range of cases. It has a high overhead, however, where a large amount of data is changed between checkpoints, as is the case with matrix operations. For these cases, a more efficient technique is desirable.

For many matrix operations, it is possible to add a checksum to the matrix in such a way that the checksum is maintained correctly at the end of the calculation. Furthermore, for some matrix operation algorithms, it can be shown that the checksum is maintained at each step of the algorithm as well. These algorithms can be made fault tolerant, with much lower overhead than checkpointing, using a matrix checksum. The overhead of making other operations fault tolerant may also be reduced by this method if the amount of data checkpointed can be reduced by the use of a checksum.

One operation that can be made fault tolerant with a checksum is the LU decomposition. The matrix has both a row and column checksum appended onto it. During the steps of Gaussian elimination, checksum
relationships for all of the elements of the matrix are maintained, although the exact relationships change from step to step. The correctness of the checksum is also maintained when it is done on a processor level instead of an element level.

When a matrix operation is done in parallel, the usual distribution of the data is block cyclic, which means that each processor holds elements of the matrix that are evenly spread throughout the global matrix. This distribution balances the work of the processors better than if each processor had a contiguous chunk of the matrix. With the block cyclic distribution, the checksum is done by adding an extra row and column of processors to the processor grid. The extra processors hold the checksums. With this arrangement, the checksum is still maintained at each step of the calculation, and a single processor failure can always be recovered from.
The sedimentary deposits of Arabia Terra have been known for some time. Satellite observations showed layered morphology of the deposits, while the MER Opportunity mission provided evidence of an ancient playa setting. The work presented in this study further postulates that the observed rocks are the remains of a once-extensive deposit. Unraveling the history of this deposit will help shed light on the development of the climate, and may have implications for better understanding the geologic history of Mars.

There are occurrences of layered sedimentary rocks (eolian sandstones), often with sulfate signatures, found around the Meridiani Planum region (the site of the Opportunity MER). Groundwater likely cemented these rocks and they even preserve sedimentary structures, like ripples, that point to liquid water being stable at the surface. The preservation of evidence for water at this site makes it of interest. The objective of this work was to see if these disparate deposits were once connected, and if so how large of an eroded volume they represent.

In order to reconstruct the eroded volume, a database of points was built. Points were first selected around the type locality of Meridiani Planum. The characteristics of these known deposits were then used to select points successively farther from Meridiani. Of particular use was the High Resolution Imaging Science Experiment, a high resolution visible light camera aboard the Mars Reconnaissance Orbiter spacecraft. These photos allowed for morphologic comparisons of the erosional patterns and layering to the type locality. After the database of points was selected, ArcGIS software was used to run several surface interpolations. Both kriging and planar surface fits were run on two different selections of data points. These surfaces were selected as they are thought to best represent the interpreted playa and dunefield depositional setting, and the inferred groundwater cementation of the deposits. Both surface interpolations yielded $\sim 7 \times 10^5 \text{ km}^3$ of eroded volume on a smaller selection of data points concentrated around Meridiani. The surface runs on the full data set yielded $\sim 2 \times 10^6$
km$^3$ of eroded sediments. While the thickness varied greatly with topography, there was up to 1 km of estimated erosion in places. These results are supported by the fact that there are pedestal craters, features where the impact ejecta preserves underlying sediments, up to 800 m high in these areas. These volumes are very large, bigger than any known sand sea deposit on Earth. As a result of these calculations, it becomes obvious that some highly effective, yet unknown, erosional mechanism was in action at some point earlier in Mars’ history. Also, if the playa depositional environment is accepted, the thickness of these deposits would indicate a long-lived hydrological system and stability of liquid water at the surface. All of these points have implications for the evolution of the climate on Mars, which may have been more transitional that the traditionally hypothesized abrupt change from warm and wet to cold and dry. The extent of these deposits argues for a period of deposition that was relatively warm yet arid.
Ga-doped Zn$_{1-x}$Mg$_x$O is of interest in a wide variety of optoelectronic applications because of the ability to tune the bandgap and work function. Historically samples with substantial Mg substitution (>10%) have been difficult to dope. Ga-doped Zn$_{1-x}$Mg$_x$O (0.02<x<0.2) films employing a digital approach to doping have been prepared by Pulsed Laser Deposition (PLD).

A target with a fixed stoichiometry of ZnO and MgO and a single Ga$_2$O$_3$ target were alternately ablated with pulses from excimer laser (KrF; 248 nm) on the fused silica substrates. Samples with different doping levels were obtained by changing the number of pulses delivered to each target in each preparation cycle. Tunable conductivity of Ga:ZnMgO is achieved. The carrier concentration and the mobility in the sample were examined with respect to the deposition parameters: ablation conditions, doping layer thickness, number and thickness of periods. The structural and electronic properties of the films were discussed on the basis of extensive XRD, four-point probe and variable field Hall measurement, while the morphology and the composition of the samples were elucidated by simultaneous AFM and Raman confocal mapping. Optical properties were also derived from UV-vis-NIR absorption spectroscopy. Based on all above-mention results, the relationship of Mg concentration and Ga doping efficiency, and the influence of Ga doping conditions on carrier concentration and mobility were discussed. The bandgap of Ga:ZnMgO was tuned by the Mg concentration, while the conductivity of this material was varied by the deposition parameters. These results serve to provide an understanding of the ability to dope and the mechanism of doping in ZnO with substantial Mg substitution, which qualifies ZnMgO for some important optoelectronics applications.
In this paper we formulate and solve the problem of model reference adaptive control for unit memory discrete repetitive processes by employing a lifting technique that allows us to view the system as a first-order multivariable plant. An adaptive controller gain adjustment algorithm in the iteration domain is given that ensures convergence of the tracking error between the output of the process and the output of a given reference model when the plant and reference model are driven by the same input.
Design and Implementation of a Remote Control System for Teleoperation of a Skid-Steer Loader over a Wi-Fi Mesh Network

Name: Christopher Joseph Meehan
Degree Program: MS
Department: Engineering – Electrical
Advisor: Kevin Moore

Emergency situations, such as mine rescue operations, would benefit significantly from the use of teleoperated vehicles. However, in an underground mine, the environment is not well suited for teleoperation. This is because an underground mine environment strongly attenuates the high frequency wireless signals required for real time video. The solution is to provide a highly redundant network backbone, composed of many wireless nodes, to relay information throughout the environment. Additionally, it is ideal to have a flexible mobile network that could adapt to reach unconnected areas and redistribute network load. In this project we consider the problem at hand and implement an autonomously adapting wireless network system, along with the conversion of a Bobcat skid steer loader to a teleoperated vehicle. The project covers the design, implementation, and evaluation of the wireless network backbone and teleoperated remote control system for a Bobcat skid-steer loader.
Performance of Alcohol Fueled Micro-Tubular SOFCs

Name: Kevin Van Galloway
Degree Program: PhD
Department: Metallurgical and Materials Engineering
Advisor: Nigel M. Sammes

Utilization of ethanol and methanol fuels in solid oxide fuel cells (SOFCs) is desirable because the storage of such fuels is much easier than hydrogen. Ceria based micro-tubular SOFCs show promise for the application of these fuels. In this study, 1.8 mm outside diameter tubes consisting of a Ni-GDC\GDC\LSCF-GDC structure are analyzed in the intermediate temperature regime between 500 and 650°C. These micro-tubular SOFCs are run using liquid ethanol and methanol fuels, as well as humidified hydrogen for performance comparison. With methanol as fuel, the maximum power densities were 700, 480, and 260 mW cm\(^{-2}\) at 650, 600, and 550°C respectively, which was higher than the power densities gained under ethanol but lower than those gained using hydrogen. The electrochemical properties of the cells run using these three fuels were investigated by AC impedance spectroscopy. The long term stability of cells using methanol and ethanol as fuel was studied under constant current conditions and the microstructures of these cells were also investigated.
Variations in the viscosity, seismic properties and other physical properties of heavy oils are poorly understood. The viscosities measured for different heavy oils can vary by orders of magnitude even at the same API gravity, which is the standard metric for lighter oils. Heavy oils are viscoelastic materials, and the bulk and shear modulus and the viscosity are coupled. Understanding what controls heavy oil viscosity will provide insight into what controls heavy oil shear modulus. Therefore, applying geochemical methods to investigate heavy oil composition in order to relate the physical and chemical properties of heavy oils are explored.

Overall, the heavy oil samples show little correlation between the viscosities or shear modulus and the API gravity, separate resin content or separate asphaltene content as measured from SARA analysis. However, the total resin plus asphaltene content collapses the viscosity and modulus values to provide empirical relations between these quantities. Also, a partial least squares regression analysis provides tight correlations for the chemical signatures from SARA analysis.

Lots of lab work has been done towards analyzing SARA composition and it is tightly related with heavy oil viscosity and seismic properties. Future work will be done towards doing lab work of heavy oil steam flooding process. And it will be related with steam rate, viscosity change and oil production amount and rate.
ADMIRE: Autonomous Dam Monitoring with Integrated Real-time Evaluation

Name: Kerri Stone  
Degree Program: PhD  
Department: Mathematical and Computer Sciences  
Advisor: Tracy Camp

Dams have a large impact on public safety in the United States. Dam failures are far reaching and may result in loss of property, loss of life, and loss of water storage. Despite this fact, dam inspections occur infrequently and are performed unevenly across the structure. As such, current dam monitoring practice is often incapable of detecting internal erosion – a primary failure mode in dams. The inability to detect internal erosion results in increased risk of catastrophic failure. This research focuses on the development of a wireless sensor network (WSN) application to autonomously and continuously monitor embankment dams for signs of internal erosion. To date, a WSN has not been used to assess dam integrity. The use of a WSN to autonomously and continuously monitor dams will improve the ability to detect structural issues before failure occurs.

This research develops ADMIRE - Autonomous Dam Monitoring with Integrated Real-time Evaluation, which will continually assess dam integrity through minimally invasive geophysical sensing techniques integrated into a WSN. ADMIRE will implement a machine learning algorithm to calculate the probability of internal erosion based on geophysical sensor measurements. Upon calculating a high probability of internal erosion, the WSN will employ a distributed algorithm to localize the occurrence of internal erosion. ADMIRE will allow for autonomous and continuous monitoring of embankment dams. ADMIRE will contribute significant technological advancements to dam inspection practice.
Cooperative Beamforming: Higher Throughput with Collisions

Name: Chris Walsh
Degree Program: MS
Department: Mathematical and Computer Sciences
Advisor: Tracy Camp

We present Cooperative Beamforming for wireless sensor networks (WSN). In the context of a WSN, beamforming uses a distributed array of independent antennas to constructively interfere radio transmissions toward a specific destination. Noteworthy benefits of beamforming include improved link qualities, increased transmission ranges, power consumption reductions, and eavesdropping countermeasures. This work extends current beamforming research by enabling source nodes to intentionally collide different packets destined to spatially different destinations into a single, multi-lobe, beamforming event. Upon reception, the collided signal can be deconstructed using blind source separation techniques to retrieve the desired signal. This allows the constructed beam to carry more than one packet and thus achieve throughputs greater than one. Beamforming poses many challenge: How does one synchronize the carrier phase of several individual radios? How does one estimate the individual transmission weights needed to shape and direct the desired beam(s)? How does one effectively select a participating subset of nodes ensuring spatial diversity and evenly distributed energy use? This poster presents the very initial work and exploration into this topic and solicits ideas and feedback.
Intelligent and Continuous Performance Monitoring: Impacts To Dam and Levee Safety Policy

Name: Minal L. Parekh
Degree Program: PhD
Department: Engineering
Advisor: Mike Mooney

Dam and levee safety can be improved by the pursuit of common goals for monitoring and management. However, dams and levees currently exist in separate institutional realms that limit the sharing of knowledge and practice. As paradigmatic examples of critical protective infrastructure, dam and levee structures present similar technical and management challenges: limited monitoring data, insufficiently developed techniques to monitor large structures continuously and densely, and limited resources to correct these shortcomings. Despite these common challenges, regulation of dam and levee safety are at different stages of “maturity” and are handled in different modes by a variety of responsible agencies. In the case of levees, national standards and policies are in the development phase; the failure of levees in New Orleans during Hurricane Katrina has generated interest in study of levee safety, of performance monitoring, and of risk assessment. In the case of dams, standards and policies are well established. Nevertheless, the public and policy makers are not necessarily showing as much interest in technical advancements for monitoring dams, due largely to the highly visible and politically significant failure of the levee systems during Hurricane Katrina. As a result, technological advancements in continuous and intelligent levee monitoring present opportunities for extending levee technical research to dams. Conversely, policies surrounding well-established dam monitoring, risk assessment, and management could inform levee safety policy. This portion of research addresses these complementarities to investigate possible technical and political bridges and hurdles to a combined vision for dam and levee safety.
A Dynamic Graph-Based Systems Framework for Modeling, of Cyber-Physical Systems Typified by Buildings

Name: Fadel Lashhab, Chang Liu
Degree Program: PhD (Lashhab), Masters (Liu)
Department: Engineering
Advisors: Kevin L. Moore, Tyrone L. Vincent

In the first part of this poster we present a framework for modeling certain classes of cyber-physical systems using graph-theoretic thinking. The cyber-physical systems we consider are typified by buildings. We show that the thermal processes associated with a building can be represented as a graph in which (1) the node variables (temperature and heat flows) are governed by a dynamic system and (2) interconnections between these nodes (walls, doors, windows) are also described by a dynamic system. In general we call a collection of such nodes and interconnections a dynamic graph and for the case of building thermal systems we observe that the steady-state behavior is equivalent to that of a static graph, so that the graph Laplacian can be used to analyze system properties.

In the second part we consider consensus networks whose nodes are integrators and whose edges are 2-tuples of real rational functions representing dynamical systems that couple the nodes. We review salient points from graph theory, including Laplacians, interconnection matrices, and consensus protocols, all of which typically involve constructs with static weights. We then generalize these notions to the case of graphs with integrating nodes and dynamic edges. We give conditions under which such graphs admit consensus, meaning that in the steady-state the node variables converge to a common value. The ideas are illustrated an example that motivated this work: the modeling of thermal processes in buildings.
Surface Reaction Mechanisms during Ozone and O₂ Plasma Assisted Atomic Layer Deposition of Aluminum Oxide

Name: Vikrant R. Rai  
Degree Program: PhD  
Department: Chemical Engineering  
Advisor: Sumit Agarwal

We have elucidated the reaction mechanism and the role of the reactive intermediates in the atomic layer deposition (ALD) of aluminum oxide from trimethyl aluminum (TMA) in conjunction with O₃ and an O₂ plasma. In situ attenuated total reflection Fourier transform infrared spectroscopy data show that carbonates and –OH groups are formed on the surface during the oxidation cycle. Chemisorption of TMA occurs primarily on the –OH groups while carbonates are the reactive intermediates, which are removed in the subsequent TMA cycle. The ratio of –OH groups to carbonates strongly depends on the oxidizing agent and the duration of the oxidation cycle in plasma-assisted ALD.
The self-induced dynamics of a vortex defect in a Bose-Einstein condensate (BEC) are well modeled by phenomenological hydrodynamics. At the macroscopic scale, vortex defects are thought to be precursory to turbulent fluid dynamics. However, at the microscopic scale, the vortex defects take on additional structure since some of their important features become quantized. While the study of vortex-tubes is most applicable for these phenomena, nontrivial dynamics also manifests from idealized line vortices and are expressed by a concise asymptotic expansion, consistent with the Euler equations, relating the local dynamics of the defect to nonlinear Schrödinger evolution (NLS). This local induction approximation (LIA) states that a bent line-vortex generates a local velocity field asymmetric in the binormal direction. These binormal flows correspond to NLS, which is a completely integrable nonlinear PDE admitting soliton solutions whose amplitude and phase controls the line-vortex curvature and torsion, respectively. Our recent work, generalizing LIA, indicates that higher order approximations offer no new dynamics in the case of a line-vortex, which is in contrast to existing results relating the dynamics of slender vortex tubes to a hierarchy of integrable dynamics. This poster will focus on the approximations results and also the geometric setting, which relates binormal flow to the nonlinear Schrödinger equation.

Name: Peng Zhao
Degree Program: MS
Department: Engineering
Advisors: Marcelo Simoes, Siddharth Suryanarayanan

A cyber-physical system (CPS)-enabled energy management system in building structures is concerned with the sensing and control of energy flows. Modern buildings exhibit a tight integration of sensing, computation, and actuation within multiple physical domains. For example, larger buildings usually contain a sensor network, with a variety of sensors that measure electric power flow, temperature, relative humidity and CO₂ levels. They control the operation of the chiller and heating systems, and may have actuators to control the air-flow into and through the building, or building access. The energy management and control system uses the sensor measurements and determines actuation; the control of which can be of a hierarchical or distributed nature. The full potential to achieve efficient energy management in building structures requires information on the thermal behavior of the building, accurate predictions of weather and building use, input from spot energy markets, equipment efficiency characteristics, and possibly access to distributed generation (DG), energy storage, smart grid technology and an evolved communication infrastructure. The efficient management of energy in building structures thus presents a ripe area for the exploration of deploying cyber resources.

Building operating systems such as heating, ventilating and air conditioning (HVAC) system, lighting, vertical transportation, etc, depend on energy from sources such as electricity and natural gas, for providing acceptable levels of security and comfort to the users. However, over 40% of energy consumed in residential and commercial buildings is associated with low efficiency heating and cooling loads. As energy prices soar concomitantly with the needs of reducing dependence on fossil fuels usage and curbing carbon footprints, building energy management system (BEMS) present an important avenue for the pursuit of end use energy
efficiency. The control and use of a BEMS may present an ideal avenue for deploying CPS that may boost the overall efficiency towards energy efficient and net zero energy building goals.

The BEMS, which is proposed for a typical medium-sized commercial office building, has three zones of interest—the electrical, heating and cooling zones. Each zone possesses local DG and renewable energy sources (RES) to offset the consumption of natural gas and electricity from the utility. Thus, the management and control of a distributed energy system at the consumer end present an issue for exploration. Due to the limited capabilities of centralized computing on large-scale distributed systems, decentralized or semi-centralized decision-making process is viewed as suitable options for employment in the cyber aspect of BEMS. A possible approach to the solution of managing distributed energy systems is through the use of multi-agent systems (MAS). The focus of current research is the optimization of energy flows in the three energy zones under a semi-centralized control paradigm aiming at minimizing energy cost.
Thin film hybrid photovoltaics, which include organic donor and inorganic acceptor components, are attractive due to higher adsorption coefficients, more desirable mechanical properties, and less expensive processing. Despite these advantages, hybrid thin films have shown limited efficiency due to poor charge separation and extensive charge recombination. While bulk heterojunction devices improve charge separation, random pathways for charge transport are interrupted resulting in losses due to charge recombination. Therefore, control of film morphology at the nanoscale is essential for further improvements in device efficiency. The present work seeks to yield well-defined architectures by selectively incorporating nanoparticles into phase segregated polymer films of poly(3-hexylthiophene) (P3HT) and poly(styrene) (PS). Reversible addition fragmentation chain transfer (RAFT) polymerization provides well defined architectures with a trithiocarbonate end group that allows for facile attachment to nanoparticle surfaces. A novel P3HT macro-RAFT agent was synthesized to provide (1) a P3HT homopolymer and (2) a P3HT-b-PS copolymer that can be readily attached to the surface of gold nanoparticles through a thiol end group. Nanoparticles modified with the P3HT homopolymer would be incorporated exclusively into the P3HT domain of the polymer film, while PS homopolymer modified nanoparticles would incorporate into the PS domain. Furthermore, it is predicted that nanoparticles modified with a P3HT-b-PS copolymer would assemble at the interface between the domains in the thin film. Therefore, several different ordered film architectures can be obtained via polymer surface modification of nanoparticles prior to incorporation into phase segregated polymer films.
Bioremediation of dense non-aqueous phase liquid (DNAPL) within a fractured bedrock setting presents unique remedial challenges compared to porous media. Little research has been done to characterize microbe transport and activity within fractured settings, especially in terms of enhanced DNAPL dissolution. This research explores the dissolution behavior of tetrachloroethylene (PCE) DNAPL in a bench-scale three-dimensional (3-D) sandstone fracture network in the presence of microbial degradation activity. Experiments are conducted using *Dehalococcoides* sp. (DHC). DNAPL dissolution in the presence of DHC is compared to dissolution behavior in the absence of DHC to evaluate the extent of dissolution enhancement. In addition, microbial kinetics, transport, and DNAPL dissolution are investigated as a function of DHC inoculation dosage. Reaction kinetics, as well as transport and delivery of microbes, are hypothesized to be affected by the complex flow patterns within a fracture network. Microbial reaction kinetics, deduced from effluent breakthrough curves, are compared to those of static batch studies. Results regarding DNAPL dissolution behavior in the presence of microbial activity from the network experiments are compared to bio-enhanced dissolution behavior results from discrete fracture experiments in order to evaluate scaling up capabilities in hopes of more efficient remediation at the field scale. Results from discrete fracture experiments have shown up to a five-fold dissolution enhancement in the presence of biodegradation.
Coal Pre-treatment and its Effects on Extractable Organic Matter

Coalbed methane (CBM) represents an increasingly important source of domestic energy in the United States comprising approximately 7.5% of natural gas consumption. The presence of biogenic methane in some CBM reservoirs, in combination with recent findings that microorganisms (both naturally occurring and lab preparations) have the ability to degrade coal and generate methane as an endproduct suggest methanogenesis may be an extant process occurring in these habitats. It follows that microbial CBM formation is an important process to understand because of its economic as well as environmental implications. However, questions still remain regarding what fraction of the coal is used by or most bioavailable to the microbial populations and whether this material can be altered to support enhanced levels of methanogenesis. In this study, we examined the effects of various pre-treatments on the extractable fraction of coal in order to better understand their influences on biogenic methane formation. Each pre-treated coal as well as an untreated preparation was exhaustively extracted with chloroform to determine the effect on extractable organic matter and the resulting hydrocarbon distribution pattern. Pre-treatment with HNO₃ had the greatest effect, increasing the bitumen content four-fold relative to an untreated sample; most of this increase resided in the asphaltene fraction, which was approximately 28-fold higher for the acid-treated sample. In contrast, bitumen content was decreased by one-half in replicate samples that were pretreated with either H₂O₂, KMnO₄, or NaOH suggesting these pre-treatments may be less effective at mobilizing biodegradable organic matter and supporting methanogenesis in situ. Results from this work will be useful in identifying pre-treatments that support enhanced rates of methanogenesis when incubated with native microbial consortia.
Building and Adding Value to a Geothermal Academy: Microbial Fuel Cell Bioengineering & Collaboration with Icelandic Biogeothermal Resources

Name: Cory D Jensen, Daniel Cano
Degree Program: PhD (Jensen), Undergraduate (Cano)
Department: Engineering
Advisor: David Muñoz, John Spear, Masami Nakagawa

Microbial fuels cells (MFC), biofuel cells (BFC), microbial electrolysis cells (MEC) and bioelectrically assisted microbial bioreactors (BEAMR) could be a part of a bioenergy wedge in the context of the so-called energy water nexus. Such systems could also be used to explore research in the areas of novel bio-material interface, consortia dynamics and integrated water treatment & chemical producing processes. Traditional mediator less MFCs oxidize substrates, perform electrogenesis via exoelectrogens and when configured to reduce an electron acceptor (i.e. anode), generate current by oxidation at a cathode. Recognition of this natural phenomenon is attributed to Potter et al. (1911) but advances that could lead to practical application were not made until much later; Kim et al. (1999 A & B), Rabaey et al. (2003), Liu et al. (2004), and Logan et al. (2006) whom suggested a first goal of scaling the technology for the treatment of water streams, respectively. We are in the process of configuring a data collection interface (Figure 1A) and construction of both a two-chamber and single-chamber microbial fuel cell (Figure 1B).
Figure 4

Contact with the University of Akureyri (UoA) in Iceland has suggested that collaboration to develop and promote MFC expertise would provide for a unique specialization in a Geothermal Academy. Common MCF research themes include; MFC architecture (i.e. engineering design), consortia characterization with traditional molecular methods & systems modeling, and investigation of chemical-biochemical mechanisms particularly those related to electrogenesis. UoA has identified consortia that have produced up to 3.2 mol-H2/mol-glucose but product dynamics that account for electrogenicity have not been characterized (Koskinen et al. 2008). Additional bioprospecting at such sites could identify exceptional exoelectrogenic species and consortia. Our poster will highlight development of a novel MFC, proof of concept results, and extensive outreach efforts since sustainable water and energy efficient technologies have witnessed a surge of research attention.
Acoustic impedance inversion for static and dynamic characterization of a CO₂ EOR project, Postle Field, Oklahoma

Name: Alana Robinson
Degree Program: MS
Department: Geophysics
Advisor: Tom Davis

Seismic inversion for acoustic impedance improved reservoir characterization of the incised valley-fill Morrow Sandstones and understanding of the CO₂ flood performance at Postle field. The use of traditional P-wave reflectivity data for identification of the Morrow Sandstone has been difficult due to the relatively low acoustic impedance contrast between the sandstone and the surrounding shale. Acoustic impedance inversion of the P-wave reflectivity data broadens the bandwidth and removes the wavelet, enabling detection of a response from the Morrow Sandstone.

Colored inversion was selected to invert the reflectivity data based on its ability to best resolve a response from the sandstone. The inversion results enabled reliable mapping of the thin Morrow Sandstone in the 3D acoustic impedance volume. A coupled inversion, using a common low-frequency model and wavelet derived from the merged datasets, was used to invert the base and monitor P-wave reflectivity volumes to enable time-lapse impedance analysis. In general, the time-lapse anomalies observed in the data correlate to the roll-out of the CO₂ flood program from south to north. When interpreted in conjunction with the production data and geologic depositional model, the patterns of anomalies enable the identification of flow pathways and baffles within the reservoir. The scale of the interpreted heterogeneities indicate the flood pattern is of near optimal dimension to sweep the reservoir. However, detailed analysis of the patterns and heterogeneities identified regions where specific well stimulations and the addition of new wells could improve sweep efficiency.

Finally, assuming the largest time-lapse anomalies correspond to high porosity sands with high permeability and likely fluid movement, the time-lapse anomaly map was used as an additional constraint in
estimating gross reservoir sandstone thickness. This addition further improved the accuracy of the prediction of gross reservoir thickness. From this map, three potential drill sites, on the edge of the current patterns, in relatively thick reservoir sandstone have been identified. In conclusion, this work demonstrates the utility and benefit of time-lapse acoustic impedance inversion for Morrow Sandstone exploration and tertiary recovery monitoring. The time-lapse monitoring also has implications for the surveillance of CO₂ sequestration programs.
Microsecond simulations of spontaneous gas hydrate nucleation and growth

Name: Matthew Walsh
Degree Program: PhD
Department: Chemical Engineering
Advisors: Carolyn Koh, Amadeu Sum, Dendy Sloan, David Wu

Despite the industrial implications and worldwide abundance of gas hydrates, the formation mechanism of these compounds remains poorly understood. Here we report direct molecular dynamics simulations of the spontaneous nucleation and growth of methane hydrate. The multiple-microsecond trajectories offer detailed insight into the process of hydrate nucleation. Cooperative organization is observed to lead to methane adsorption onto planar faces of water and the fluctuating formation and dissociation of early hydrate cages. The early cages are mostly face-sharing partial small cages, favoring structure II, however larger cages subsequently appear due to steric constraints and thermodynamic preference for the structure I phase. The resulting structure after nucleation and growth is a combination of the two dominant types of hydrate crystals (structure I and structure II), which are linked by uncommon $5^{12}6^3$ cages facilitating structure coexistence without an energetically unfavorable interface.
Disclaimer: The abstracts and related information printed in this booklet are taken as-is from the submissions of each presenter, and were edited only to fit the format of this booklet. Any typographical errors, misrepresentations, or other miscommunications are the sole responsibility of the presenter.

Please visit the GSA website at: organizations.mines.edu/GSA