College of Science BSMP Poster Session 1

14 july 2016

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1

Connecting an EV Charging Station to a Mesh Network through an IoT router

Eusebio Neto, Joao Curcio, Nathan Buch, Dr. Kevin Jin

CS

This is a pilot project to connect an experimental EV Charging Station in a laboratory environment to a mesh network maintained by Silver Springs Networks using their IoT router, which allows them to connect to many IoT devices and manage them in real time. The purpose of this connection is to extract meter data from the charging station and store it in the IoT router to be later accessed by Silver Spring Networks on their backend software.
There's also a side project to run an x86 executable under a Linux ARM environment to extract data from EV charging stations that are already installed on campus.

2

UFarm IIT - Smart Sustainable Farm

Bernardo Abreu, Cristhian Carvalho, Kevin Jin, Nathan Buch, Jason Engstrom, Jimmy Shah, Farshogar Umrigar

CS

UFarm is an urban farm, which aims to eliminate the constant need of human supervision. It contains solar panels, sensors, actuators and other devices that help the farm to manage itself. The objective of this project is to develop a scheduling system for water irrigation for the UFarm. Initially, a connection between a Central Control Station and the valves, that would perform the irrigation, was established through the use of Radio Frequency signals. Then, the devices responsible for receiving the Control Station signals were programmed to act according to these signals, controlling the valves. A software was developed to run on the Control Station, scheduling the irrigation process by sending the necessary signals to the valves. The final part of the project was to conduct tests with the devices and a valve before implementing them on the field.

3

Predicting the Molecular Mechanism of Anthocyanin-Induced Insulin Sensitivity

Alice Duarte Mendon'a Telles, Amanda Costa Spolti, Bing Xie, David D. L. Minh

Chemistry

Insulin resistance is implicated in the development of Type 2 Diabetes, the most common type of diabetes. Several flavonoid subclasses found in berries, such as anthocyanins, have been associated with a reduction in risk of type 2 diabetes. In this study, we have identified possible molecular targets through searches of online chemical databases and through software that can predict similar binding sites.

4

Implementation of a Force Field term to increase precision of docking simulations and prediction of binding free energies on systems with a receptor and a rigid ligand.

Allan M. F. de Amorim, Luiza P. P. Machado, Laurentiu Spiridon, David Minh
Chemistry

Molecular dynamics and molecular docking simulations prove themselves to be very useful tools on many functions, such as predicting the effectiveness of chemical components, e.g., pharmaceuticals. The current work presents a proposal of improvement for the method of simulating receptor-ligand systems to obtain the binding potential mean force (PMF) for specific poses and, consequently, the free energy associated with the binding reaction. By adding a force field argument to the calculation of the ligand's binding PMF, which restrains the molecule in a certain pose based on the interactions with the receptor, we expect to reduce the computational effort to get the results and more precise estimations for the ligands energies. This force field term is added to the equation that calculates the Binding PMF for the ligand's sampled molecules and implements the routine developed for the docking simulation. To prove the precision of the method, different systems receptor-ligand were tested based on their crystal structures. With these simulations on different systems, we try to get significant results with good convergence estimates and correlation with previous data to prove the force field is an efficient improvement on the predictions.

5

Bacterial Genome Sequencing using Oxford Nanopore

Anne Caroline Mascarenhas dos Santos, Robert R. Butler III, Jahna Soomer-James,' Jean-Fran'ois Pombert
Biology

Sequencing the genomes of bacteria is important to identify essential features of these microorganisms, for example hard to characterize metabolic pathways and/or novel virulence factors. The field of microbial genomics has advanced greatly over the last decade with the advent of high-throughput sequencing. However, assembling genomes using data obtained from short-read-based technologies (e.g. illumina) is complex and can produce incomplete genomes whenever repeated sequences are present. Longer reads are needed to solve these repetitive elements, and while spanning the gaps can be done by PCR followed by Sanger sequencing, this process is cost-prohibitive and time consuming. Recently, high-throughput long-read technologies have been developed, the first from Pacific Biosciences, which works great with small genomes but requires both large amounts of input DNA and the absence of contaminants. This can be problematic with hard-to-culture microorganisms, which is often the case for pathogenic bacteria and/or species growing as part of complex microbiomes. The latest technology being developed at Oxford Nanopore works differently and does not rely on DNA synthesis. Instead, bases are read as single-stranded molecules are ratcheted through pores. Due to the use of these nanopores, the amount of input DNA is lower than for PacBio and the technology is more robust to contaminants. However, nanopore sequencing is still at the prototype stage and not yet ready for market release. In this research project, we tested the ease of use of nanopore sequencing for microbial genomics.

6

Morphology and valence state of the high proton conductors BaZr(1−x)Y(x)O(3−δ) (BZY) and Ba Zr(x)Ce(0.8-x)Y(0.2) O(3−δ)' (BZCY)

Ayla Leitao and Alison Felix
Physics

The study made comprehends the sol-gel synthesis and characterization of the proton conductive electrode materials BaZr(1−x)Y(x)O(3−δ) (x changes from 0.1 to 0.9) and metal doped BaZr(0.8−x)Ce(x)Y(0.2)O(3−δ),(x changes from 0.1 to 0.7), by using XRD, SEM, BET and XAS techniques in order to analysee the morphology and valence state of the material. Both materials have applications on fuel cells production, working as proton conductive electrodes or electrolytes.

7

High energy ball milling synthesis of SnO2/Graphite composites anode material for Lithium-ion batteries

Beatriz Almeida Liberino Tavares Silva, Yujia Ding, and Carlo Segre.

CS

SnO2 ' um material usado para confec''o de 'nodos de baterias Ion-L'tio como um substituto de maior efici'ncia para os materiais amplamente utilizados. O processo de ball milling foi usado para cobrir as mol'culas de grafite com as nano part'culas de SnO2 e para homogeneizar a mistura. Os processos de XRD e SEM foram usados para caracterizar o sample quanto ao seu tamanho e qualidade. Por fim, avalia''es eletroqu'micas quanto ao tempo de carga e descarga foram feitas para contatar os resultados.

SnO2 is a material used in order to confection anodes of lithium ion batteries as a more effective substitute for the commonly materials used currently. The ball milling process was done to cover the graphite molecules with the nano particles of SO2 and also homogenize the system. The process of XRD e SEM were applied in order to characterize the sample according with its size and quality. Then, electrochemical evaluations were done within the charge and discharge time to analyze the results of improvement of the battery.

8

SafeChicago

Breno Figueiredo Nunes, Giovane Vieira Bonifacio, Iury Cristovao Esquarcio Dutra, Sou Cheng T. Choi

Math

"SafeChicago is a tool intended to translate crime data gathered by the City of Chicago into friendly information. This tool is made possible by the conjunct effort of the Brazilian Scientific Mobility Program (BSMP) and the Illinois Institute of Technology (IIT).

Although an incredible city, Chicago has a huge problem regarding violence. Despite plenty of data related to crime, the City of Chicago's Data Portal is not quite efficient in displaying this data in a user-friendly way for its community. Having it exhibited in overwhelming tables, the simplest of visualization queries can be a difficult picture to comprehend for the users. In this project, our team develops a tool that enables users to visualize and comprehend Chicago's crime data. The gathered data was treated and used to generate an interactive filled-map with filtered crime data and a heat-map containing theft data, since it is the most common crime in Chicago. The team will also calculate the violence index of a certain region by comparing it to a crime standard. The calculation results informs the user of safety in specific locations of the city. The tool presents a solution for visualization of crime data and will make it easier for users to stay safe in the streets of Chicago."

9

Leverage of Gaussian Process Regression and Sequential Sampling

Bruno Laiber de Pinho, Fabricio Trentini, Gabriela de Oliveira Macedo, Jos' de Oliveira Lima Neto, Luciano Marreiro Abilio

Math

The Gaussian Process (GP) or Kriging Model is one of the most popular regression methods in

modeling spatial data and computer simulation output. This research is trying to optimize a code for GP Regression in order to minimize its running time. The process itself consists of predicting new output values based on previously given data. A correlation matrix is calculated in the process and with the help of estimated parameters and selected models, new points may be evaluated as an output. Cook distance, hat matrix and leverage calculation are some of the tools used to check if the model found complies with the requirements for the prediction. This entire process may be repeated several times, creating the Sequential Sampling, which is a technique used to decrease sampling costs by reducing the number of observations needed.

10

Analysis of exon edited dystrophin rods f42|54 and f43>55 for future exon skipping therapy for Duchenne Muscular Dystrophy (DMD)

Carolina Niemczyk Brito and Nicholas Menhart

Biology

Duchenne muscular dystrophy is a fatal genetic disease that affects every 1 in 3500 male births and is caused by de novo mutations in the dystrophin gene. The most common type of defect seen (~70%) is a deletion of one or more exons leading to a frameshift which eliminates translation of' dystrophin protein leading to the manifestation of the disease. In the past few years, exon skipping therapy was proposed as a therapeutic alternative for DMD. This strategy silences additional exons in order to restore the reading frame and thus dystrophin expression. Some exon edited options, such as exon skipping 51, have proceeded to clinical trials in humans. Unfortunately, the repaired protein produced by exon skipping is NOT the entire dystrophin protein but contains a deletion consisting of the patient's initial defect as well as the therapeutically skipped exon. Clinical data from related condition, BMD, suggests that these exon skipping therapies will have different clinical outcomes. However the nature of this is unknown in most specific cases. The objective of this study is to evaluate the end products of such an alternative repair of the same underlying defect. This test system involves the defect □exon44-53, which can be repaired by skipping either exon 43 or 54, to produce the targets f42|54 or f43>55, respectively. We cloned and produced these proteins in order to determine which option is the most beneficial for DMD patient taking in consideration the stability and structure of these end product proteins.

11

Electrospun silk fibers: preparation, characterization and post-treatment

Cesar Emiliano Hoffmann da Silva, Pedro Carneiro do Val, Lais Akemi de Almeida Sasaki, Naiwei Chi, Rong Wang

Chemistry

Spider silk is a biopolymer with great mechanical properties.Among the seven types of silk produced by Nephila clavipes, dragline silk is the strongest due to the combination of random coil conformation matrix along with highly organized β-sheet domains.Spider silk fibers are difficult to harvest in nature because spiders cannot be raised at dense population due to their solitary and predatory characters.To overcome this obstacle, various methods have been explored to produce silk fibers.In this study, electrospinning technique was applied to fabricate fibers from silk proteins extracted from the milk of genetically engineered goats.The objective of the research is to generate well-aligned,strong and stable fibers with submicron-diameter.We examined fibers produced from silk protein with concentrations ranging from 80 to 200mg/mL.With the increase of protein concentration, the fiber elasticity, ultimate stress and stability increase and the fiber alignment is better, however the fibers are much thicker.Fibers with 150mg/mL silk content outperform fibers prepared at other concentrations.To further improve the quality of the fibers, silk fibers were electrospun and post-treated with 75%(v/v) ethanol vapor for 1, 3 and 6 hours,

respectively.It was observed that the diameter of the fibers decreased with the duration of the ethanol vapor treatment. In comparison to non-treated fibers, 1-hour treatment didn't cause significant difference in the mechanical properties of the fibers, whereas 3 or 6-hour treatment increased the fiber elasticity and ultimate stress dramatically.FTIR spectroscopic study indicated that the ethanol vapor treatment led to apparent increase of peaks at ~1622 and ~1518 cm-1, which are characteristic of β-sheet conformation in silk proteins.Thus, ethanol vapor treatment has the effect of prompting β-sheet formation in the fibers.Further modification of the post-treatment is needed to improve the strain of the fibers.

12

Network Routing: Algorithm Design and Analysis

Dianny Gomes Dos Santos, Igor de Oliveira Nunes, Italo Guedes Almeida Silva, Joao Henrique Gon'alves Veras,' Renan Fernandes Silva, Wellington Rodrigues Pereira, Sanjiv Kapoor (PI)

CS

Software Defined Networking (SDN) is an emerging networking architecture that aims to abstract the actual ossified physical network to make it dynamic and adaptable, centralizing the control of the network's flow into remote controllers. Its programmability allows us to change rules and network behavior based on its topology, state, and business requirements. In the traditional approach for the routing process, ' which corresponds to selecting paths to forward packets in a network ' each pair of hosts uses a single path to send data. The goal of this work is to investigate the benefits of using multiple paths on specific high'bandwidth SDN networks. Simulations were performed in an emulated environment, with virtual hosts and switches, and the results show significant improvement in the network throughput.

13

Measurement of LogP Parameters in Cloud Computing Environments

Daniel G. Bueno, Erik S. Candeia, Bruno P. Masquio, Douglas N. de Oliveira, Caio V. Ortu, Mauro D. L. Tosi, Eunice E. Santos, John Korah, Vairavan Murugappan

CS

In recent years, cloud computing has increased in popularity by providing various on demand services such as infrastructure, platform, storage and software services. The opportunity to scale resources easily has made cloud computing a cost effective computational platform for the scientific community. Most of the scientific applications utilize distributed/parallel algorithms. Therefore, understanding the performance of these parallel algorithms on cloud platform becomes critical. Traditional parallel models such as Bulk Synchronous Parallel (BSP) and LogP are primarily designed for a cluster environment and do not consider virtualization or resource sharing. LogP, a widely used distributed memory model provides an efficient way to design and analyze parallel algorithms in cluster environments. In this project, we conducted initial mesaurements of' LogP parameters for cloud platforms under varying conditions. LogP model has four key parameters: Latency (L), the time taken by a message to travel between two processors; Overhead (o), the time spent by the processor in sending/receiving a message; Gap (g), time interval between two consecutive messages; Processors (P), number of processors. In this project, we used Apache CloudStackTM, an open source cloud platform, to record initial effects of factors such as virtualization and network traffic, which are relevant to a number of synthetic and real world applications (such as video streaming), on LogP parameters.

14

An Open-Source Web Interface for Computer Aided Drug Design

Emilia Fortes Rocha, Luiz Fernando Cieslak, Pedro Henrique Morais Delmondes

Chemistry
Scientific software is useful to automate researchers' daily job, but often they are non-intuitive to use as their focus is on functionality and performance instead of good user experience. Scientists, then, need to be trained to use this kind of software, specially if they are not familiarized with computer technologies as most of these softwares have installation and run processes that require command-line interactions. This project aims to develop an easy-to-use and user-friendly interface for AIGDock (Algorithm Grid Docking), a docking web application developed by Dr. Minh's research group. The GUI is being developed using Agile Methodology, with twice per week meetings to collect feedback from science students and mentors. The preliminary results are new software's screens, with enhanced functionalities and user journey, a style guide for future changes on the GUI and documentation to help future developers that will work on this project. By making easy-to-use scientific software, this project aims to facilitate and improve the efficiency of AIGDock users. Also, by having an user-friendly interface, the application will spread out, reaching different users across the world.

15

Experimental and Theoretical Study of Nanofluid Coolants - Coolant Testing Device

Fabio Kalat; Giovane Gouveia Lopes Da Silva; Elena V Timofeeva

Chemistry
"Cooling systems play an important role in the functionality of a variety of devices such as refrigerators, engines, and microprocessors. With miniaturization of many of those devices the thermal loads per surface area increase, which requires development of more efficient coolants and systems with an improved global heat transfer coefficient. To address this issue we are developing nanofluid coolants, which are a suspension of solid nanoparticles in a base fluid. Solids have much higher thermal conductivity than liquids, while liquids enable convective heat transfer, and combination of the two enables fluids with superior heat transfer coefficients.
In this project we have designed, built and tested the coolant testing device that enables side-by-side comparison of the cooling abilities of the different coolants.' A series of graphitic nanofluids were tested and compared to commercial antifreeze coolant, which was used as a base fluid. We reviewed several types of heat exchangers, and designed our own variation of it addressing our design restrictions: the small volume of fluids available. A 3D model of our device was created with the Autodesk Fusion' software. Further we have machined the device, calibrated it for different temperatures and flow rates, and tested it in different modes with base fluid and multiple nanofluid coolants. From the collected data, the most favorable conditions for the optimization of heat transfer fluid' are obtained."

16

Parallel Computing and GPU Processing Approaches to GAIL Routines

Fabio Ricardo Araujo da Silva, Renan Luigi Martins Guarese, Fred J Hickernell

Math
This research is meant to find ways to improve the performance of GAIL (Guranteed Automatic Integration Library) routines through solutions in Parallel Computing and GPU processing. GAIL is a MATLAB library that brings together a suite of algorithms for integration problems in one and many dimensions, and whose answers are guaranteed to be correct, using Monte Carlo and Quasi Monte Carlo methods. We intend to show how parallelizing GAIL routines would help their performance. Different methods have been tested in the course of the project, such as Matlab's Parallel Computing Toolbox, integrating Java classes to Matlab and Julia's performance compared to Matlab's. Preliminary results have led to a new approach and change of course. By using GPU processing we achieved faster results that will assist the library in a better manner. A Summary

report of the results obtained during our tests will be discussed.

17

Generalizing some GAIL routines to handle integrals over circular regions

Felipe Sousa de Andrade and Fred J. Hickernell

Math

This project aims to generalize some GAIL (Guaranteed Automatic Integration Library) routines to handle integrals over other regions. The routines that can be generalized are, namely, cubMC_g, cubSobol_g and cubLattice_g, which were initially able to use Monte Carlo or quasi-Monte Carlo methods to compute integrals over a d-dimensional box with uniform measure and over d-dimensional space with Gaussian measure. This project focuses on two different transformations that are useful to accomplish the project goals: box-to-ball transformation, and normal-to-ball transformation. Both transformations can be used to get a set of points uniformly distributed on a ball, with the first one starting with a set of points uniformly distributed on a box and the second one with a set of points normally distributed on a d-dimensional space. Two similar transformations that can be built are box-to-sphere and normal-to-sphere transformations, which will be able to get a set of points uniformly distributed on a sphere (the boundary of a ball). Box-to-ball and normal-to-ball transformations have been developed, implemented inside the cubMC_g routine, tested and improved for efficiency. They are to be implemented inside the other routines and the box-to-sphere and normal-to-sphere transformations are to be developed and implemented inside the same routines. All these integrals can be applied to electromagnetism, among other fields of study. They can be used, for instance, to compute the electric field inside and outside a ball or a sphere with a charge distribution.

18

Helicopter ground resonance model including a 2-dimensional mass spring damped system'

Frederico Monteiro Pinheiro Cassaro,' Joao Victor Costa Cavalcante Dantas, Pedro Henrique Souza De Albuquerque Goncalves, Paulo Muraro Ferreira,' Xiaoxia Xie

Math

The purpose of the present work is to analyse the effectiveness of linear damping in preventing the Ground Resonance of a 2-dimensional Helicopter Model. The Lagrange equation were used to achieve a 6x6 non-linear system for equations of motion for the x and y direction displacement of the helicopter fuselage. Using Taylor expansion and neglecting higher-order terms, the system were linearized, and then simplified to a 4x4 linear system after applying the Coleman transformation. Adam113 and ODE45 MATLAB's' functions were executed and and a stability analysis of the system were performed.

19

Engineering Profections: Technical Improvements at MRCAT

Gabriel Cascaes, Jeniffer Arvelos, Pedro Mantovani, Joshua Wright

Physics

Sector 10 at the Advanced Photon Source is a state of the art beamline consisting of high precision equipment with exacting standards. New developments for the beamline require interdisciplinary specialists designing groundbreaking devices with the highest standards to reduce any errors or systemic noise concerns that would be unobservable to any standard laboratory setting. Our team developed from the ground up electronic devices for beam position monitoring using a split ion chamber, mechanical structures for rapid beamline configuration, and computer programs designed to automate the entire set up procedure. Each project came to full term with a final product now currently in use at a DoE laboratory further pushing MR-CAT to maintain

spectroscopic superiority.
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20

Exploring the Performance Trade-offs in Image Retrieval using SIFT Algorithm

Gabriel L. A. Costa, Michael A. D. Sampietro,' Mateus L. Teixeira, L. H. Velloso, John Korah, Eunice E. Santos

CS

The scale invariant feature transform (SIFT) is widely used in a number of image processing applications such as object recognition, panorama stitching, and image matching. Even though SIFT is effective, its processing scalability still remains a challenge due to the large number of features generated for each image.' Although there are parallel versions of SIFT such as PCA-SIFT, GPU SIFT, Optimized GPU SIFT and Multicore SIFT, they require large and expensive computational resources when scaling to truly large and dynamic images databases. SIFT's speed and accuracy performances are greatly affected by the size of the scale space and number of keypoints used. Increasing the scale space's size and number of keypoints will result in better matches but requires additional computation time and memory allocation. In this project, we examined the SIFT algorithm and recorded' SIFT's performance on an image testbed by varying the number of octaves used. An initial implementation of a web image crawler was used to generate the image test bed.

21

Silver Spring Networks Devices Network Measurement

Gabriel N. Crispino & Leonardo dos Anjos Teteo

CS

This project had the goal to test the peer-to-peer network connection between two devices developed by Silver Spring Networks: the Field Service Unit(FSU) and a portable IoT streetlight device. During the course of this project, several tests were made on the IIT campus to see how they communicated in different conditions, to provide SSN more data about this for future projects and developments.

22

Experimental and Theoretical Study of Nanofluid Coolants

Ivan Frutu'so Almeida, Maira de Paula Nunes

Chemistry

Cooling systems play an important role in the functionality of a variety of devices such as refrigerators, engines, microprocessors. As those devices become smaller, the heat flux per surface area increases as well, calling for better cooling systems with improved heat transfer coefficient. To address this challenge in this project we focus on the experimental and theoretical study of promising nanofluid coolants, which are the suspensions of nanomaterials in liquids. Solid materials have high thermal conductivities, while liquids have convective heat transfer mechanism. Due to the combination of two phases (liquid and solid), nanofluids, suspension of nanoparticles, present advanced heat transfer properties. However, the nanoparticles expressively increase the viscosity of the coolant fluid, which causes increase in pumping power penalties. Our project focused on the development of new surface oxidation methods for graphite nanoparticles and formulation of nanofluids in a commercial antifreeze as a base fluid EG/H2O (50/50 - solution of ethylene glycol and water).' The results on characterization of nanoparticles from three different synthesis routes (scanning electron microscopy (SEM), thermogravimetric analysis (TGA), X-ray diffraction analysis (XRD), Fourier-transform infrared spectroscopy (FTIR) and Raman

spectroscopy), and characterization of thermo-physical properties of nanofluids at different particle concentrations and temperatures are reported and compared to performance of the base fluid performance.

23

Porting Gail Routines To R

Jo'o Mateus Santana da Cunha, Marcela Ribeiro Basso and Ramon Oliveira dos Santos

Math

The Monte Carlo method is used for getting numerical results based on random sampling. It is mainly used in three distinct problem classes: optimization, numerical integration, and generating draws from a probability distribution. The algorithms we have are in Matlab language, which requires a license to use it. Therefore, we started to porting the routines to R. In order to port these routines, we have used Octave and RStudio softwares and a 'R Reference' document that has Matlab codes and its respective in R. We ported an algorithm called MeanMC_CLT, which is a Monte Carlo method to estimate the mean of a random variable and also another one called MonteCarloAvgDist, which computes the Euclidean distance matrix among pairings given two sets of locations. Furthermore, we started working on unit tests on R using the RUnit and testthat packages. This topic was chosen because we realized that it is important to have these routines in other programming languages. Besides, R is an open source program and more accessible among statisticians and computer science majors.

24

Exon skipping strategies and Duchenne Muscular Dystrophy (DMD): Characterization and analysis of edited dystrophin rods f42|56 and f42|58 to optimize future exon therapy

Joao Mateus Vieira Dutra and Nick Menhart

Biology

Duchenne Muscular Dystrophy (DMD) is the most common and severe genetic disorder that cause muscular dystrophy. The high incidence of the DMD, affecting around 1 in 3600 male births, is due to the size of the dystrophin gene, the largest human gene. DMD is generally caused by the exons deletions which create a shift in the reading frame leading to a defective transcriptional product. Specific removal of an exon from a defective DMD gene can stabilize DMD gene product leading to a semi-functional dystrophin, reducing the severity of the disease. However, in order to create a stable and semi-functional DMD gene product the gene defect needs to be related to the therapeutically exon skipped. Different deletions in the DMD gene are associated with different clinical outcomes and the efficacy of this treatment vary greatly between the different mutations. This work involves the characterization of dystrophin in different exon deletions for the clinical relevance of the exon skipping therapy. We generated the exons deletions and the repairs and we characterized them by measuring the stability of its product, determining the most stable and functional dystrophin. The experiments were conduct using edits f42|56 and f42|58 (deletions of exons 43 to 55 and 43 to 56, respectively). A defective □44 can be manipulate and repair by skipping the □43 or □45, however different deletions generate different products which are not always usable for clinical treatment. The study of the deletions will help to determine which exons edits can be used for the therapy and which repairs are more promising for future clinical use. Determining the efficacy of this therapy will help optimize future clinical treatment and trials, making the therapy more specific for the specific gene mutation of the patient.

25

Nonequilibrium Path-Ensemble Averages' for Symmetric Processes

Joao Paulo Castro Zerba, Luiz Matheus Barbosa Santos

Chemistry
We developed a path-average estimator for symmetric protocols. The estimator was implemented in python and used to estimate free energies and potentials of mean force from single-molecule pulling simulations.

26

Controlling Chaos via Feedback Method

Joao Rafael de Paula

Math

Since 1963 the study of the dynamical aspects of differential equations has had many different approaches and discoveries after Edward Lorenz presented his work 'Deterministic Nonperiodic Flow' with conclusions that would later be proved and lead to various studies. The system of nonlinear differential equations presented by Lorenz has a great dependence on the initial conditions presenting different results for the smallest changes on those and this condition is called chaos. New researches and published papers about the subject have shown more systems similar or derived from the Lorenz system that show comparable behaviors but have not been as studied. Although mathematically this subject has been very interesting, for engineering chaos is not a desirable thing and unpredictable results need to be controlled or avoided. Looking at this approach, this research aim to apply the feedback control method presented by M. T. Yassen on 'Chaos control of Chen chaotic dynamical system' on the Lorenz-like and Chen-like systems to control chaos showing the results with mathematical proofs and numerical iterations using the software MatLab.

27

Simulating an Antimatter Gravity Interferometer

Lucas Maia Rios, Lucas Neves Abrantes, Yuri Rossi Tonin, Daniel Kaplan, Derrick Mancini, Melanie Cornelius, Tom Roberts

Physics

"Does antimatter fall up? The science-fictional idea of antigravity is now being taken seriously by a number of researchers around the world. If antimatter is found to behave in a way other than the expected, it will fundamentally change our view not only of gravity but of the nature and evolution of the Universe.

The purpose of this experiment is to determine whether antimatter is subject to gravity or antigravity. In order to do so, a muonium beam will be directed through a three-grating interferometer inside a cryostat. As the muonium atoms pass through the gratings, an interference pattern will form. Gravitational or antigravitational effects will cause the beam to either 'fall up' or 'fall down,' which will shift the interference pattern, and measuring this shift will allow for a direct observation of antimatter gravity.

'

Our group's main goal is to improve and provide documentation for an existing computer simulation of the optics of a three-grating interferometer, written in the C and C++ programming languages. The program takes into account design parameters such as the distance between the gratings and their relative positioning, and physical parameters of the beam such as its width and the speed of its constituent particles, in order to generate a simulation of the optical paths of the diffracted beam and of the interference pattern at the third grating. It is also possible to account for interactions between the beam and the physical structure of the device.

By varying the relevant parameters, we can predict how different interferometer designs affect the outcome of the experiment, so as to optimize the device before construction. Understanding the source code of the simulation and documenting how the physical theory is appropriately

implemented will make it possible for future research students to improve upon the accuracy, generality and computational time efficiency of the program, and pave the way for new functionality."

28

Towards the prediction of allostery, cooperativity and functional selectivity using unbound protein structures to compute the bounded state distribution.

Lucas Rodrigo Ferreira Fraga, Tha's Balestra da Silva, Chen Li, Trung Hai Nguyen, David D. L. Mihn.
Chemistry

Adenylate kinase (ADK) is an enzyme that plays an important role in the process of cellular energy transformation. Its main function is the production of adenosine monophosphate (AMP) and adenosine triphosphate (ATP) from adenosine diphosphate (ADP) and because of its importance, the ADK system is largely used to study protein's allostery and cooperativity. The use of the probability density curve from the protein's unbound state to obtain the bound state faster could be done in order to save computational time. The goal of this article is to prove that the use of binding potential mean force (BPMF) to reweight the unbound probability curve to obtain the unbound state is valid. The reweight process is done, firstly, using the YANK software and methods of Principal Component Analysis (PCA). The angles between different points of the system were also extracted and provide the histogram with all the possible molecular configurations. Using the histogram, the probability curve can be created. The following calculations are based in order to obtain parameters to reweight the unbound curve from the unbound system with ADK.

29

Barium Titanate Zirconate synthesis by Sol-gel method

Lucas Viana Costa, Yujia Ding and Carlo Segre
CS

In this present project it is reported an alternative method for obtaining a non-Pb piezoelectric ceramic Ba(ZrxTi1-x)O3. Samples consist in light-colored powders synthesized in a Sol-gel process using Barium Nitrate, Zirconium (IV) oxynitrate hydrate and Titanium tetrachloride solution, Citric acid and Ethylene glycol. After the synthesis it was characterized by X-ray diffraction (XRD) using General Structure Analysis System (GSAS) and Scanning electron microscope (SEM). The results show compositions remarkably close to expectations with minimal impurities. This work demonstrates a new and promising recipe for obtaining Barium Zirconate Titanate (BZT) in a safe and harmless procedure.

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30

Tracking Frequency Gauge and Advanced Frequency Counter

Luiz Felipe Manke
Physics

General Relativity predicts that all objects accelerate identically in gravitational field, regardless of their composition (Einstein's famous Principle of Equivalence). In this research, a precision nanotechnology atom-beam interferometer needs to be developed to be used with an antimuon beam at Switzerland's Paul Scherrer Institute to prove or denied General Relativity. To do this, is important to analyse and simulate studies as well as design and test of an alignment system with picometer precision. This last objective can be achieve by a tracking frequency gauge (TFG) that uses lasers to measure picometer and subpicometer. This past Summer, we worked with the TFGs and also with the AFC (Advanced Frequency Counter) and were able to get some good

results for a such short time. After taking some data for a few days and analysing it, it was possible to measure 5 picometers. It is a exelent start, but it need a lot of improvment to reach 1 or less picometer so it can be used in the experiment.

31

WITHDRAWN

32

Experimental and theoretical study of nanofluid coolants

Marcelo Rocha and Yago Braun

Chemistry

"Cooling systems play an important role in the functionality of a variety of devices such as refrigerators, engines, microprocessors. As those devices become smaller, the heat flux per surface area increases as well, calling for better cooling systems with improved heat transfer coefficient. To address this challenge this research project focuses on the experimental and theoretical study of nanofluid coolants, which are suspensions of solid nanomaterials in liquids. This study was focused on the theoretical study of promising graphitic nanofluids which are reliant on the percolation heat transfer mechanism.

In our project we developed a computational model using MatLab software to evaluate the percolation threshold, i.e. the concentration of particles at which continuous heat conduction paths are formed, resulting in superior thermal properties. We have investigated the effect of particle morphology on the percolation threshold in 2D and 3D simulations.

At the same time computational fluid dynamic simulations (CFD) utilizing the COMSOL software were performed to study the effect of nanofluid properties on the efficiency of heat transfer. Simulations were conducted for a coolant testing device/heat exchanger, which was designed, build and tested by another members of our class. The results of CFD simulations we compared to the experimental results.

33

CHARACTERIZATION OF THE ROLE OF HIS257 OF V. CHOLERAE FLAVIN TRANFERASE ApbE

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Biology

The aim of this project is to characterize the role of the catalytic residue Histidine 257 in the recently discovered family of flavin transferases, ApbE. The importance of this enzyme relies on its activity, incorporating the FMN cofators to the subunits NqrC and NqrB of the main ion transporter in Vibrio cholera, the sodium dependent NADH dehydrogenase (Na+-NQR). Na+-NQR is the first enzyme of the respiratory chain in many pathogenic bacteria and its activity is related to many physiological functions. Our preliminary results showed that the conserved histidine residue 257 has an important catalytic role for ApbE. Here, we produced and characterized several mutants of this residue, including H257G, H257K and H257E and found that they displayed low flavin transferase activity, indicating that His257 is essential for the function of ApbE.

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34

Exon skipping therapy for Duchenne Muscular Dystrophy (DMD) treatment: Construction and Analysis of the Dystrophin Rod Edit f44|54 and f44|56

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Biology

Duchenne muscular dystrophy (DMD) is a form of muscular dystrophy that causes muscle degeneration, leading to paralysis and premature death, among other consequences. Although

this is a genetic disease, it is in general not inherited, but rather arises' from de novo mutations in the Dystrophin gene. This is because those afflicted do not survive to reproductive age, and since it is the largest of the human gene, it is a large target for de novo mutations. These mutations lead to incorrect translations of the protein Dystrophin and affects 1 in 3500 males. Dystrophin stabilizes the cellular membrane, thus, when it is missing or defective the results are muscular deterioration similar to 'early aging'.' There is no current curative therapy, and the current standard of care aims to control the symptoms and maximize the life quality and expectancy. This is not very successful, and DMD patients generally rely on wheelchair at age of 12-15 and die at 21-25. A new therapy, based on exon skipping was submitted to trial in 2008 and appeared to be successful. This technique consists in skipping extra exons around the patient's mutation, essentially enlarging the patient's defect to get a more stable protein than the naturally affected. In most cases there are alternative ways to skip extra exons, resulting is differently edited proteins, with possibly different stabilities. This work consisted of the production and analysis of 2 members of such alternative repairs, f44|54 (fusion of the exon 44 with 54 skipping the exons in between) and f44|56 (fusion 44 to 56). These edits are alternative repairs to DMD defects consisting of De46-52 (missing exons 46 to 52), De46-54 and De45-54. By' testing the stability of the proteins containing these edits, we can determine optimal exon skip repairs for those patients and, hopefully, contribute to some advance in the care for DMD research. Both of the fragments were successfully sequenced and led to the protein analysis step.

35

Synthesis and characterization of Li-Ion battery cathode material

Michele Borba Pavao, Shankar Aryal and Dr. Carlo Segre.

Other

The Li-rich cathode Li1+x (Mn5/8 Ni2/8 Fe1/8)1-x O2 was synthesized for several values of x between 0 to 0.3 using a sol-gel method, which uses citric acid as chelating agent. The structural, morphological, and electrochemical properties of the prepared samples were characterized by various methods. Using X-ray diffraction (XRD) it was possible to identify impurities in some of the synthesis. It has also been performed morphological test with scanning electron microscopy (SEM), which showed very small particles. In coin cells test, it was analyzed the samples NMF-M2, which has x=0.3, and NMF-M3, with x=0.15, and, for the first two cycles, the NMF-M3 presented better results than NMF-M2, discharging for 9 hours and 42 minutes, what represents approximately' 97% of the calculated time, while the other one discharges for 7 hours and 15 minutes. This low-cost, Fe-based compound prepared by the sol−gel method showed goods results, which are close to the expected theoretically, and it has potential to be used as a high capacity cathode material for Li-ion batteries.

36

Eigenfunction Analysis of General Positive Definite Kernels

Tanner Johnson, Greg Fasshauer, Fred Hickernell

Math

In this work we present several ways of realizing the reproducing kernel Hilbert space (RKHS) associated with a general positive definite kernel. Mercer's theorem tells us that every positive definite kernel admits an eigenfunction expansion. This allows us to study the properties of kernels in general by studying the eigenfunctions and eigenvalues they're composed of. This naturally leads to an associated differential operator defined in terms of the eigen-pairs. We show that given a positive definite kernel a differential operator whose domain is its RHKS is uniquely prescribed and vice versa. Thus opening up the theory of differential equations to be applied to RHKS's. Finally, we present several ways of constructing kernels from general eigenfunctions and

eigenvalues.

37

Heston Stochastic Volatility Modeling in GAIL - Guaranteed Automatic Integration Library

Tianci Zhu, Xiaoyang Zhao, Fred J. Hickernell

Math

The Guaranteed Automatic Integration Library (GAIL) is a suite of algorithms that includes Monte Carlo methods for multidimensional in- tegration and computation of means. GAIL can generate an appropriate number of samples needed to meet the desired tolerance. Our group works on construction of the financial module of GAIL.

Stochastic volatility models play an important role in improving the accuracy of pricing financial derivatives. There are several well-known stochastic volatility models: the Hull-White model (1987), the Scott- Chesny model (1989), the Heston model (1993) and the SABR model (2002). The Heston model is of particular interest to us since it is one of the most widely used stochastic volatility models.

In this project, we apply the Quadratic Exponential (QE) algorithm to simulate the volatility process and use the Broadie-Kaya scheme (2006) to discretize the asset price process. However, the Broadie-Kaya scheme will involve infinity terms when v, the volatility of the asset price's volatility, goes to 0, resulting in incorrect answers given by the algorithm. We use a change of variables to correct it and extend the applicable range of the original algorithm to the case when $v \approx 0$.

To improve the efficiency of the algorithm, we use the Brownian Mo- tion generator in the GAIL to generate the normal distribution needed in the algorithm. We test the algorithm by setting $v = 0$, such that the volatility of the asset price is a deterministic value and the result shows that the asset price process generated by QE scheme is within the error tolerance when compared with other simulation scheme, such as the geometric Brownian Motion.

38

Adaptive Variance Reduction for IID Monte Carlo Simulation in GAIL - Guaranteed Automatic Integration Library

Tianpei Qian, Fred J. Hickernell

Math

The Guaranteed Automatic Integration Library (GAIL) is a Matlab library that provides algorithms for integration problems in one and many dimensions, and whose answers are guaranteed to be correct. Among all the algorithms, there is a 2-stage algorithm that is based on IID Monte Carlo simulation. In the latest released version of this library, there is still no option for users to adopt variance reduction techniques when using this algorithm, although common variance reduction techniques such as control variates and antithetic variates can greatly speed up the simulation if carefully applied. Therefore, we propose a 3-stage algorithm that allows the user to add in control variates or antithetic variates while still guaranteeing the correctness of the answer. Moreover, the new algorithm can automatically select the optimal variance reduction techniques when multiple methods are suggested by users. This algorithm proves much more efficient for problems with at least one good variance reduction technique suggested by the user and essentially no worse than the original algorithm when none of the techniques are effective.

39

Internet of Things and Smart Advertising Application

Rafael Silveira, Marcus Seixas, Kevin Jin,Nathan Buch and Jason Engstrom

CS

With new technologies and the use of Internet of Things, people are looking for new solutions that

can change the world as we know. Our focus in this project was to design an innovative way of advertising for smart cities. With the help of an intelligent camera and an IoT router, we have the opportunity to create a new approach for companies that want to advertise. Different advertisements will be seen depending on how many pedestrians are being detected and counted by the Placemeter Sensor. Then the IoT Router will be running scripts that will download data from the Sensor and change the advertisements being shown on a monitor. With this data we can create different rates for advertising pricing, regarding the number of people passing through the area.