Commonwealth Computational Summit

Poster Competition

29 Posters

7 Universities (15+ Departments)

16 Big Computing, 9 Big Data, 4 Future Technologies

# Use of HPC to analyze changes in gene expression during fruit fly spermiogenesis

Sepideh Dadkhah, Biology, UKy

- ## Research Category
  - Bio-informatics, NGS, Development, Spermiogenesis, JAK/STAT Pathway

- ## Description of Research
  - This study has compared transcriptional profiles of testes in which JAK/STAT signaling has been genetically arrested prior to individualization during spermiogenesis to testes from wild type flies using RNA-seq methods.
  - The main goal of this project is to characterize the events downstream of JAK/STAT signaling in spermiogenesis and more specifically to determine the mechanism by which JAK/STAT activation regulates individualization, a later stage in spermiogenesis where 64 individual spermatids are formed from a 64-interconnected spermatid bundle.

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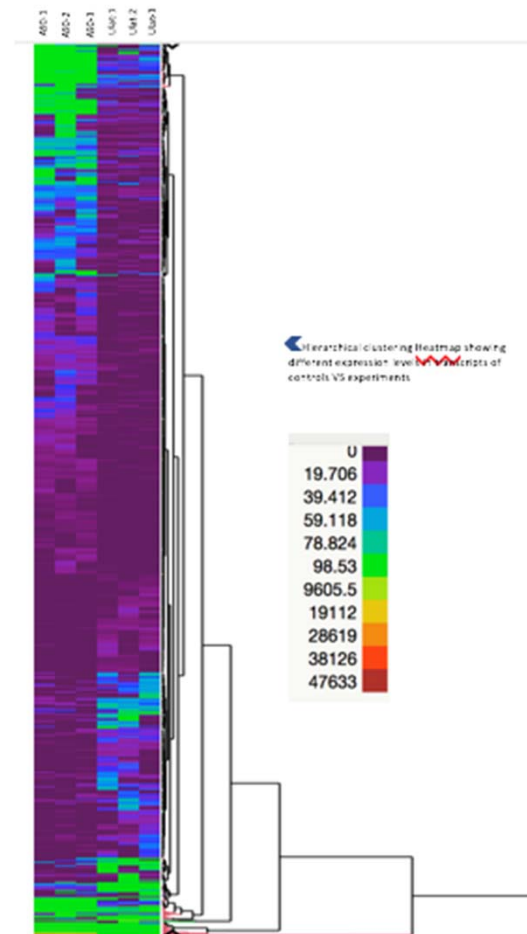
Computational Materials Characterization, Discovery, and Design with High Performance Computing

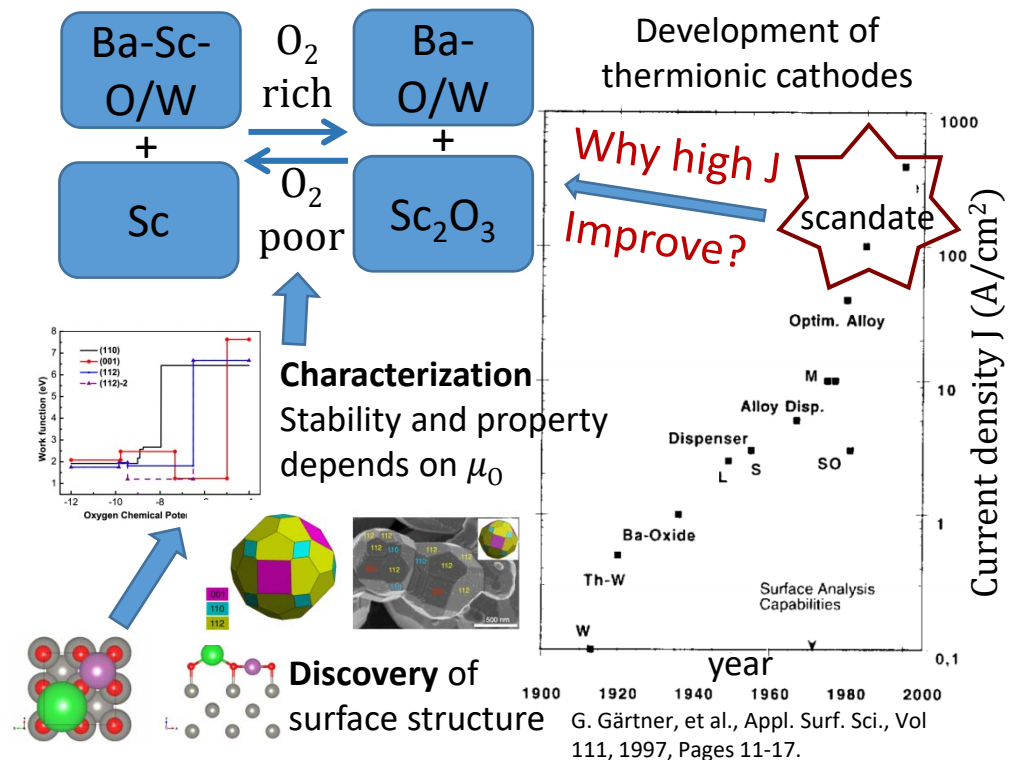Qunfei Zhou, Department of Chemical and Materials Engineering, University of Kentucky

- **Research Category**
  - Big Computing/HPC

- **Description of Research**

  - This project demonstrates how supercomputing are used for discovery, and characterization of emitting materials in thermionic scandate cathode, both to uncover the underlying mechanism for superior electron emission density and solve a long-standing problem, which provides guidance for design of improved and novel cathodes.
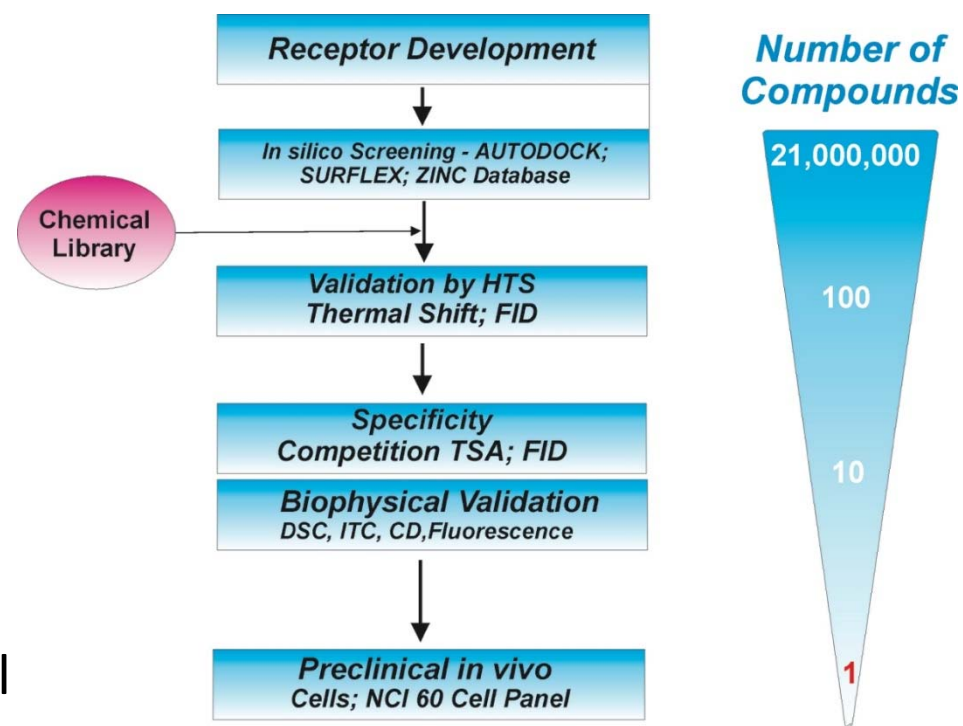
- Table of Content Graph

Characterization
Stability and property depends on μ_0

Discovery of surface structure

Development of thermionic cathodes

Why high J Improve?

scandate

G. Gärtner, et al., Appl. Surf. Sci., Vol 111, 1997, Pages 11-17.

Structure-based Drug Discovery: Computational Virtual Screening

Robert Monsen, Biochemistry & Molecular Biology, University of Louisville Medical School, Louisville KY

- ## Research Category
  - Big Computing
- ## Description of Research
  - Receptor-based virtual screening of millions of compounds against cancer/disease related proteins and nucleic acid targets for the design of novel therapeutics.
  - We also use molecular dynamics simulations to probe the 3D conformational landscape in order to create receptors that allow for more accurate docking.

Chemical Library

Receptor Development

In silico Screening - AUTODOCK; SURFLEX; ZINC Database

Validation by HTS Thermal Shift; FID

Specificity Competition TSA; FID

Biophysical Validation DSC, ITC, CD,Fluorescence

Preclinical in vivo Cells; NCI 60 Cell Panel

Number of Compounds

21,000,000

100

10

1

Integrative Computational Modeling for Developing Means to Manipulate Biological Cells and for Solving Complex Engineering Problems

Yu Zhao, Ph.D.

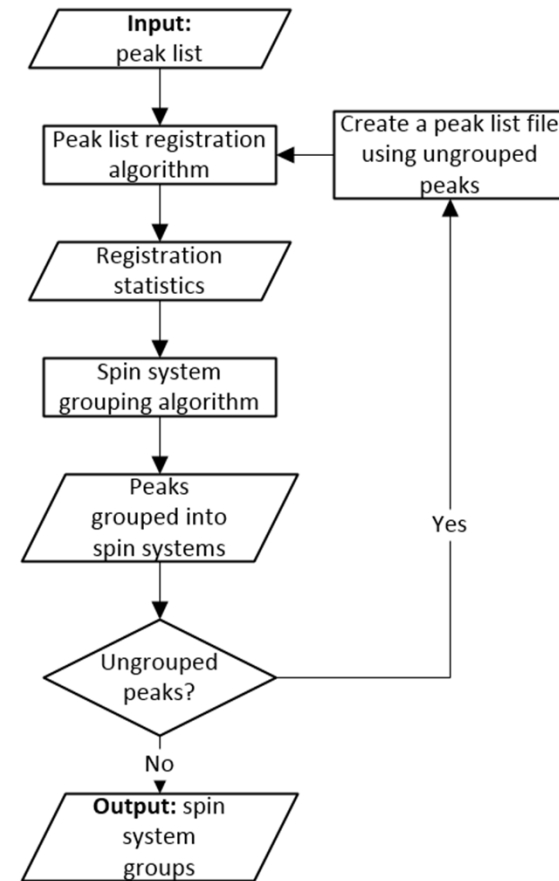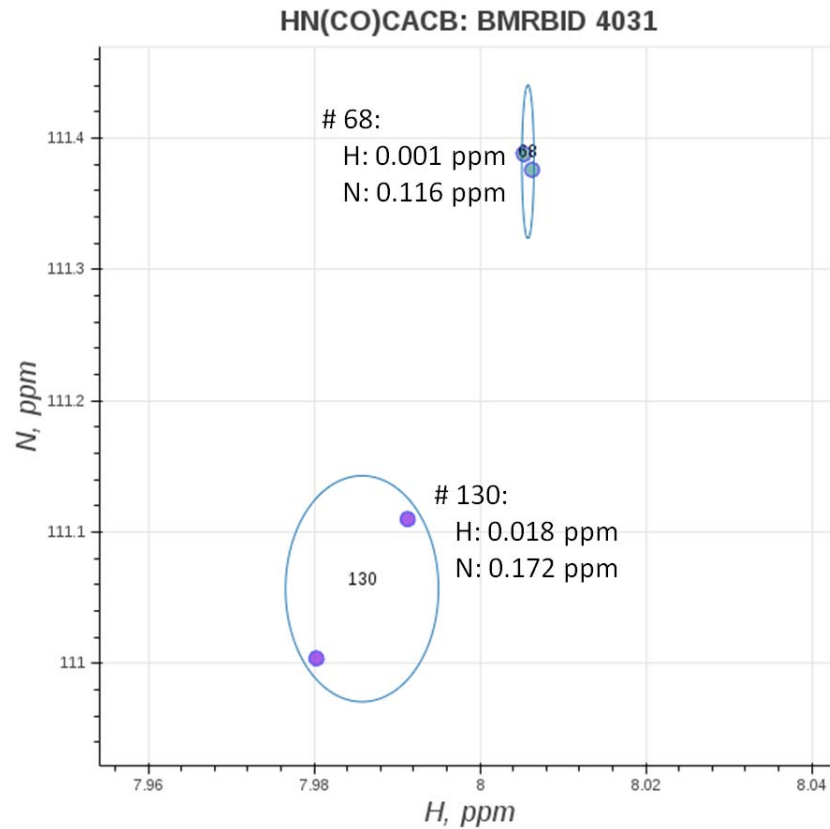**F. Joseph Halcomb III, M.D. Department of Biomedical Engineering, University of Kentucky**

- ## Research Category
  - ### Big Computing/HPC

- ## Description of Research
  - This presentation shows how to effectively use computational modeling to provide means for examining current theory and developing new theory in order to obtain better understanding of experimental observation. It also shows the power of computational modeling for solving complex engineering problems in an integrative way.

- ## Compelling graphic/visualization
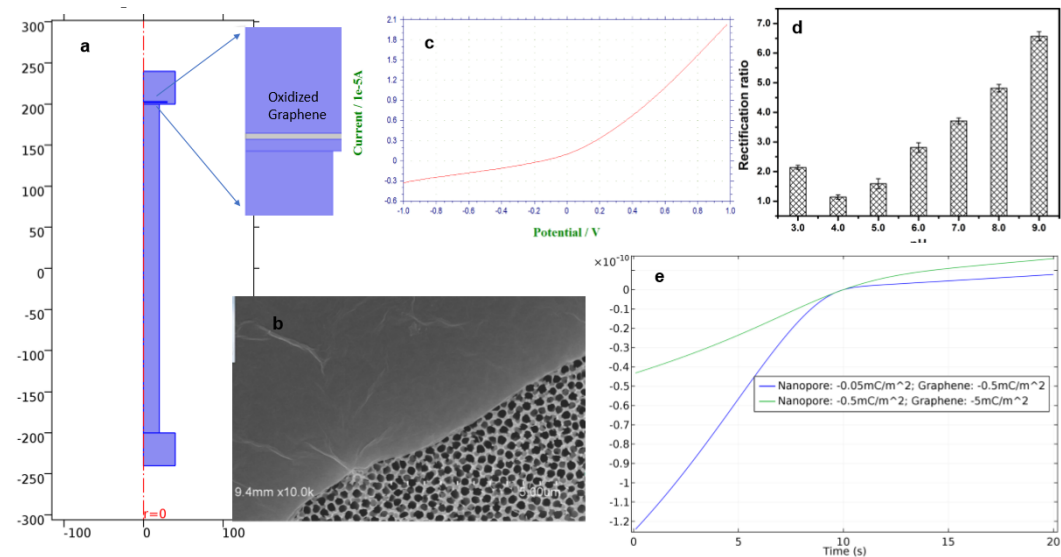
Registration and grouping algorithms in protein NMR derived peak lists and their application in protein NMR reference correction
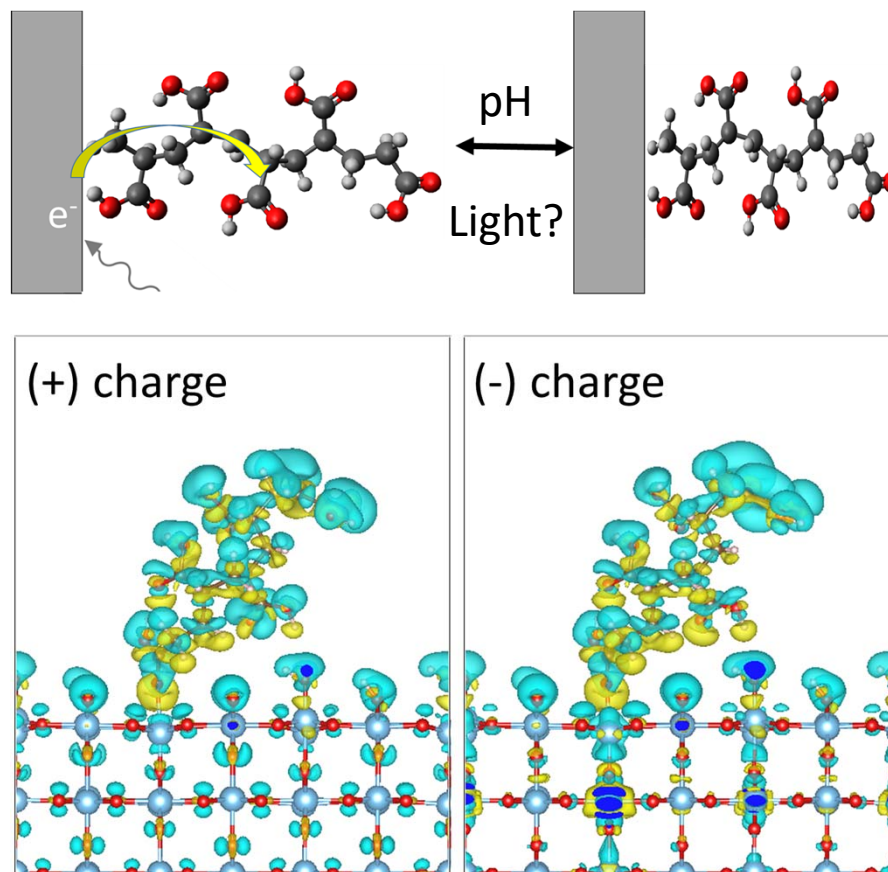

HN(CO)CACB: BMRBID 4031

68:
H: 0.001 ppm
N: 0.116 ppm

130:
H: 0.018 ppm
N: 0.172 ppm

N, ppm

H, ppm

Input: peak list

Peak list registration algorithm

Create a peak list file using ungrouped peaks

Registration statistics

Spin system grouping algorithm

Peaks grouped into spin systems

Ungrouped peaks?

Yes

No

Output: spin system groups

- Registration algorithm allows inferring registration statistics for a single peak list that has multiple peaks per spin system.
- Grouping algorithm allows grouping peaks into spin systems within a single peak list and can handle multiple sources of variance that is present within experimental data sets.

Investigation of Photo-Responsive Titania Surfaces

Evan Hyde, Department of Chemical and Materials Engineering, University of Kentucky

- Big Computing/HPC – DFT Quantum Mechanical Calculations
- Photocatalytic TiO_2 was modeled in solution using Density Functional Theory with implicit solvation to predict the strain of adsorbate molecules from photoexcitations of light. Calculations will be used in the design of a selective, photo-responsive membranes of PAA on TiO_2.

pH

Light?

e^-

(+) charge

(−) charge

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The Effect of Inlet Pulsations on Liquid Jet Atomization

Kyle Windland & Prashant Khare, Department of Aerospace Engineering & Engineering Mechanics, University of Cincinnati
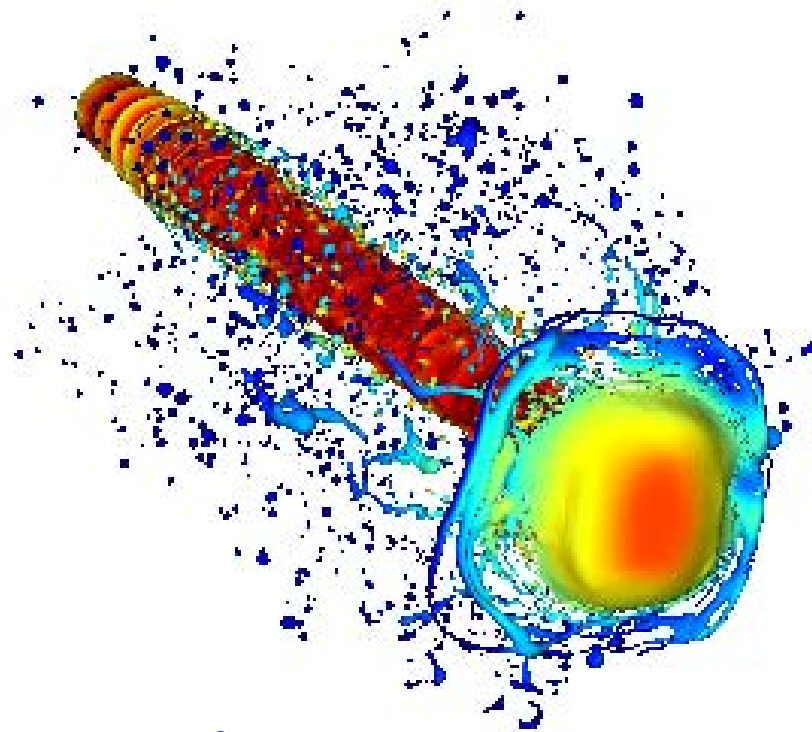
Research Category:

- Computational Fluid Dynamics

Objectives

- Elucidate the physics underlying the primary atomization of liquid jets.
- Investigate the effect of inlet pulsations at a range of frequencies from 0-100 Hz on the atomization process.

X-component of the velocity of the jet, U_i (m/s)

| 0.0 | 12.5 | 25.0 | 37.5 | 50.0 |

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Evolution of Barred Galaxies in Spinning Dark Matter Halos: High Resolution N-body Simulations at DLX
Angela Collier, Physics, University of Kentucky

- Big Computing
  - Astrophysics Computation/Theory
- Galaxy Morphology and Evolution
  - This project attempts to explain the Hubble Fork. Why do galaxies have such different morphology? How do DM halos effect this evolution?

- Hubble Fork:
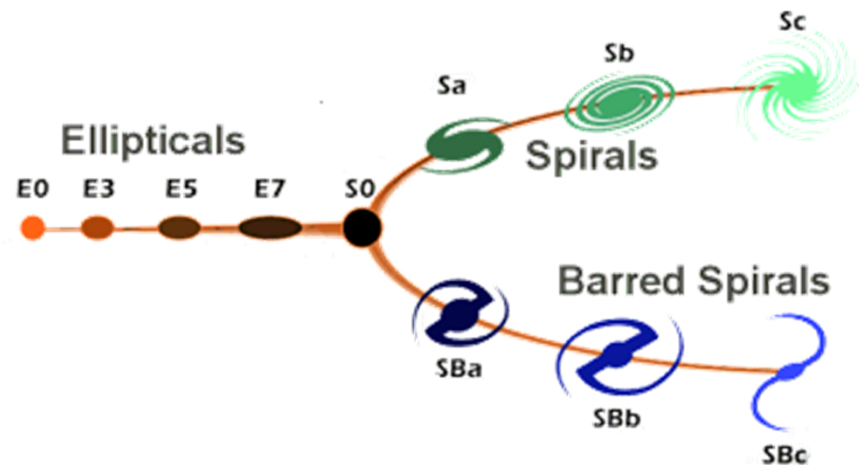
Utilizing Nvidia GPUs for Waveform Analysis for the Nab Experiment

David Mathews, Physics and Astronomy, University of Kentucky

- Big Computing

The Nab Experiment at Oak ridge requires very rapid but precise analysis of waveform data to extract accurate measurements of physical phenomena. Traditionally real-time analysis of waveforms has been handled by FPGAs. This project demonstrates that Nvidia GPUs are capable of real-time analysis with more complex filtering techniques than the traditional FPGA method can provide.

Convolution Rate Comparison (MB/s)

i7-6700k	3.15
GTX 1070	14456.7
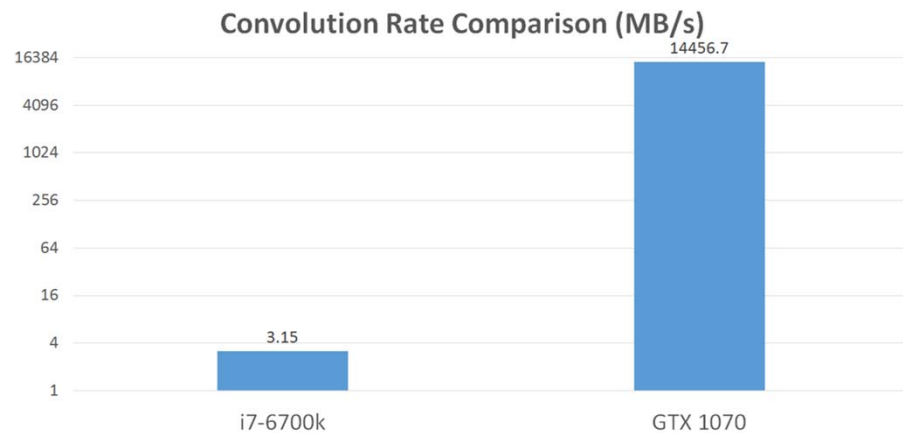
Parallelization of a Three-Dimensional Full Multigrid Algorithm to Simulate Tumor Growth
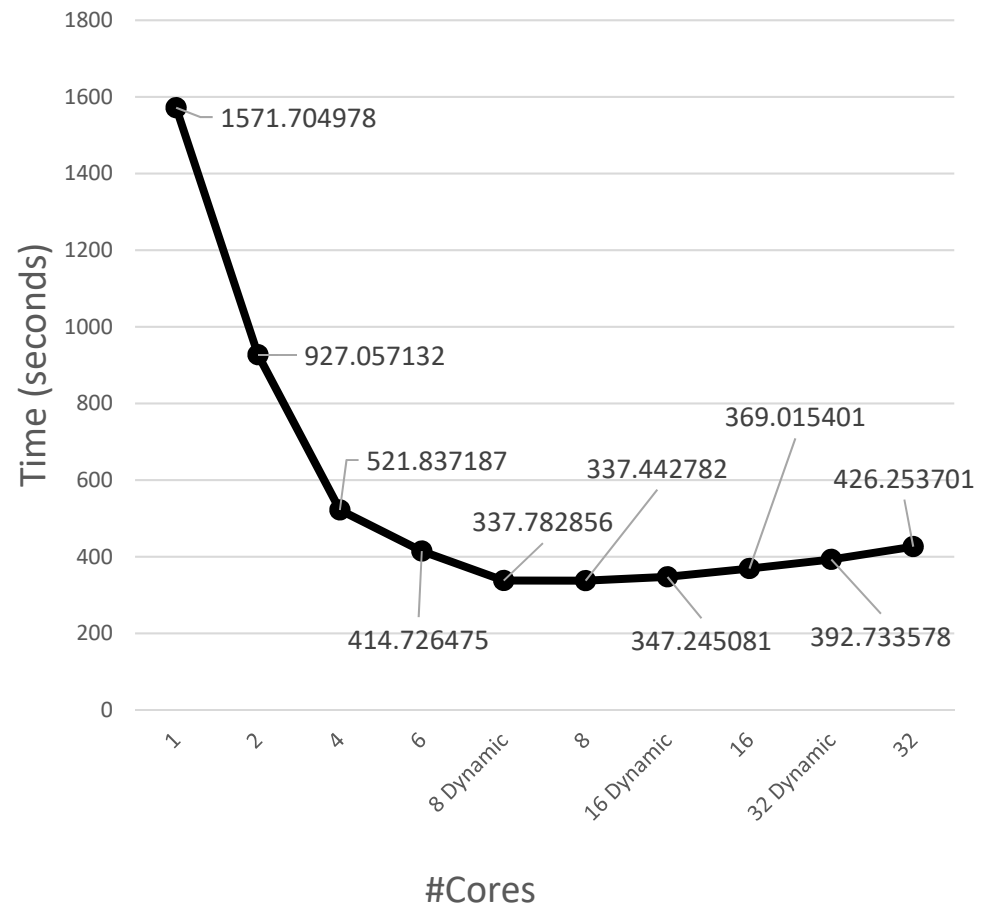
Dylan Goodin, Dept. of Bioengineering, University of Louisville

- ## Research Category

  Parallel Processing/HPC

- ## Description of Research

  We present the performance gains of an openMP implementation of a fully adaptive nonlinear full multigrid (FMG) algorithm to simulate three-dimensional multispecies desmoplastic tumor growth on computer systems of varying processing capabilities.

Time (seconds) vs **#Cores**

#Cores	Time (seconds)
1	1571.704978
2	927.057132
4	521.837187
6	414.726475
8 Dynamic	337.782856
8	337.442782
16 Dynamic	347.245081
16	369.015401
32 Dynamic	392.733578
32	426.253701

# Discovery of sex-specific regions in a salamander genome

Nataliya Timoshevskaya, Department of Biology, UK

- ## Research Category
  - Bioinformatics

- ## Description of Research
  - The large size and complexity of salamander genome presents serious computational challenges at almost every step of traditional genomic analysis
  - This project will present our approaches to assembly and downstream computational analyses of the assembled salamander genome, in particular identification of sex-specific genomic regions

Axolotl genome

32 Gigabases = 10x

BIG GENOME = = BIG PROBLEMS

VS
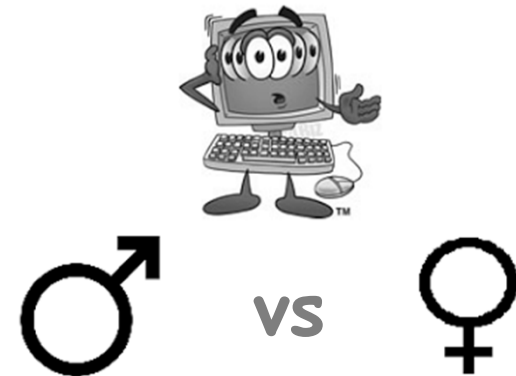
Formation of Supermassive Black Holes in the Early Universe: High-Resolution Numerical Simulations of Radiation Transfer Inside Collapsing Gas

Yang Luo, Department of Physics & Astronomy, University of Kentucky.

Astrophysics

- radiation hydrodynamics

Numerical simulation of the formation of supermassive black holes

- This project will help to understand how the black hole is formed at the beginning of the universe.

- It will help to explain the observations of high redshift qusars.

- The early formation of a dense core in the center of a dark matter halo.
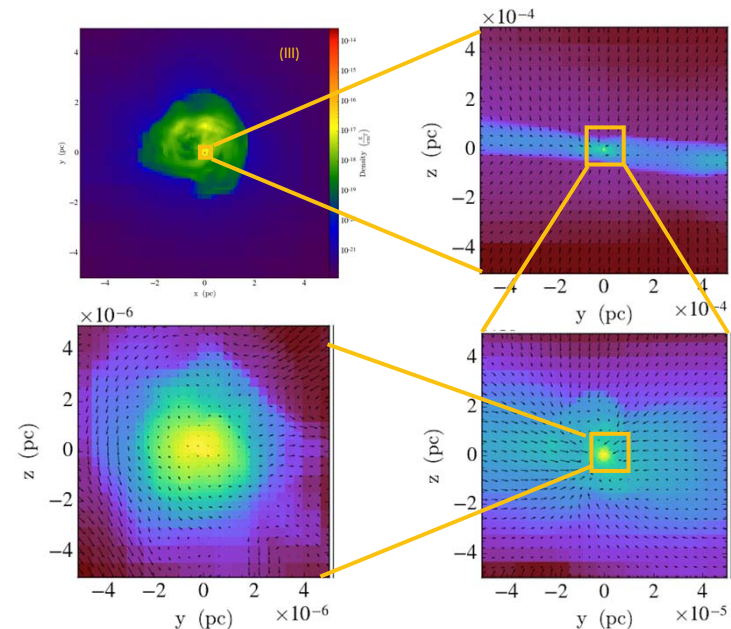
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Spectroscopic and Computational Characterization of Lanthanum-Mediated C-H and N-H Bond Activation of Amines

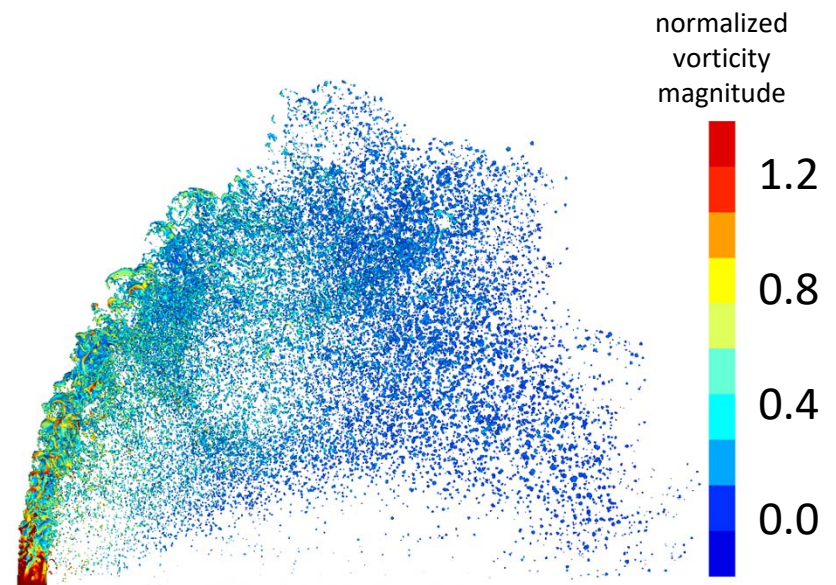**Silver Nyambo: Department of Chemistry, University of Kentucky**

- My goal is to uncover the requirements that affect C-H, N-H and C-C bond cleavage or their transformation into other bonds in alkanes and amines and shed new light on metal-mediated hydrocarbon transformation into value-added products.

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High-Fidelity Simulations of Water Jet in Air Crossflow

Austin Johnston, Department of Aerospace Engineering and Engineering Mechanics, University of Cincinnati

- ## Research Category
  - Computational Fluid Dynamics

- ## Description of Research
  - Investigate detailed physics underlying liquid jets in crossflow configurations.
  - Develop models to predict the statistical behaviors of resulting droplets

- ## Compelling graphic/visualization

normalized vorticity magnitude

1.2

0.8

0.4

0.0

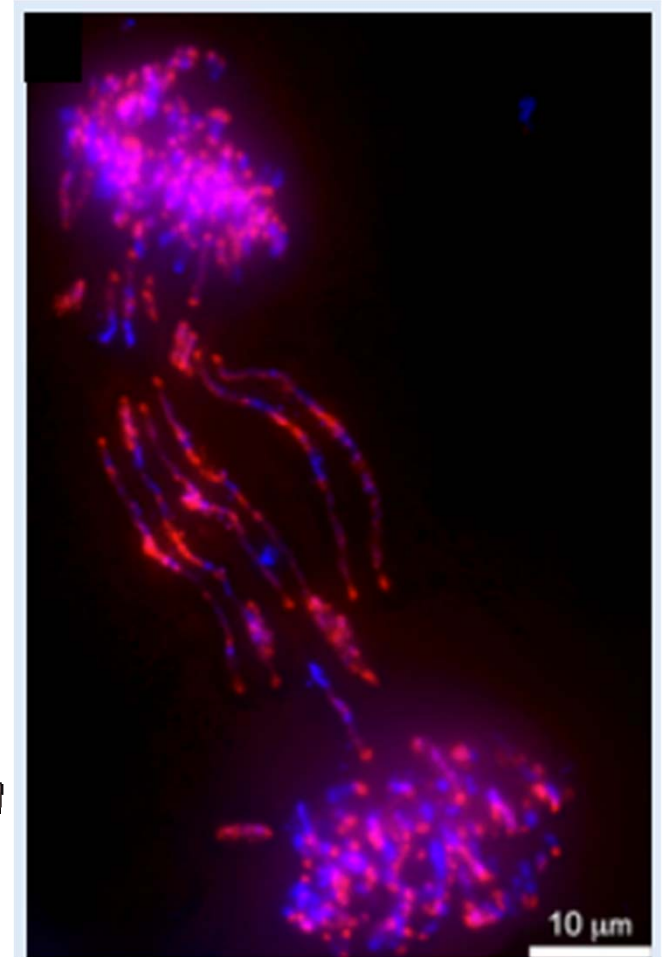1st Annual Commonwealth Computational Summit – October 17, 2017

The lamprey genome: Illuminating genomic change across eons and embryogenesis

Courtney Waterbury, Department of Biology,
University of Kentucky

Big Computing

The lamprey genome provides unique insights into both the deep evolutionary history of vertebrate genomes and the maintenance of genome structure/integrity over development


10 µm

Dark Matter Halo Mass Function From HPC N-body Simulations

Da Bi, Department of Physics & Astronomy, University of Kentucky

- ## Research Category
  - Big Computing

- ## Description of Research
  - In previous simulation work, it is found that there is an low-mass end excess comparing to the theoretical Sheth–Tormen slope in dark matter halos mass function. We used GIZMO to check this. The results implied this low-mass end excess may be an artificial effect, which depends on the random density fluctuation in a finited sample volume.

- ## Compelling
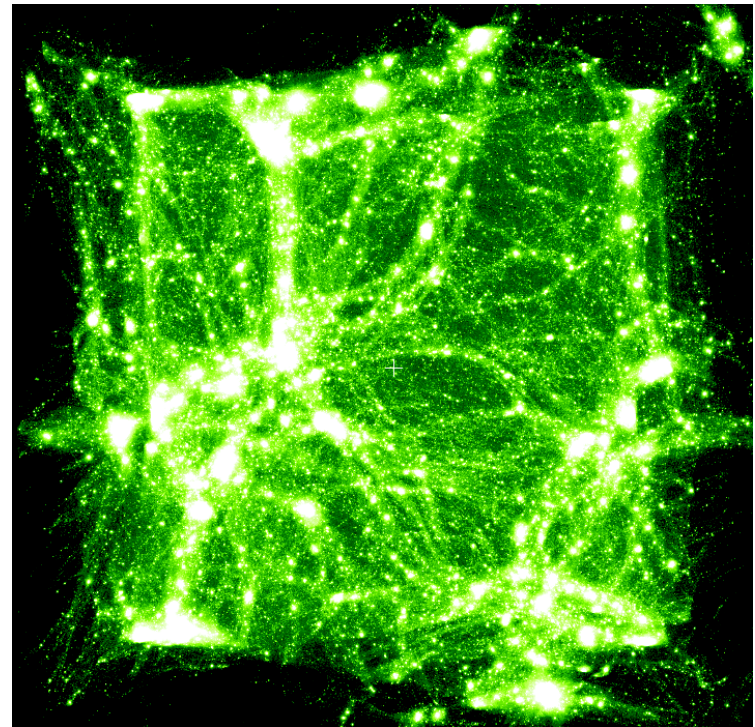
Snapshot of 20Mpc box N-body cosmology numerical simulation at redshift 0.

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Evolution of Bias in Human and Machine Learning Algorithm Interaction

Wenlong Sun, Olfa Nasraoui, Patrick Shafto,
Dept. Computer Science & Computer Engineering, University of Louisville

- Research Category
  - Machine Learning/Big Data

- Description of Research

- Develop an iterated-learning framework to study the interaction between machine learning algorithms and users.
  - The process by which people select information to label.
  - The process by which an algorithm selects the subset information to present to people.

- Compelling graphic/visualization
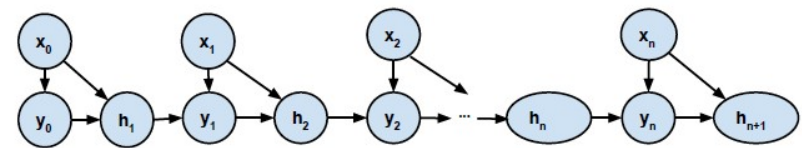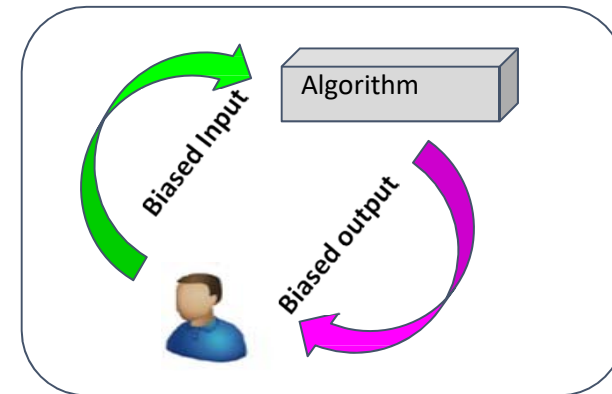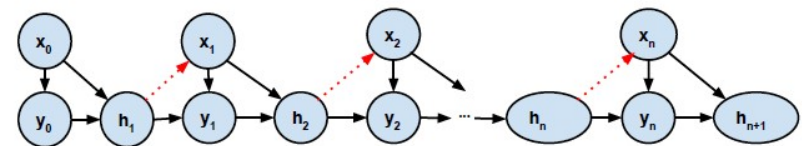
Grading Complex Tasks through Crowdsourcing

Lingyu Lyu, CECS, University of Louisville

- Research Category
  - Truth Discovery in Crowdsourced Data
- Description of Research
  - Examines how spammers effects the accuracy of grading complex tasks via crowdsourcing
  - Build model combing spam removing and de-biasing to improve performance of crowdsourcing algorithms
  - Optimize the number of graders to reduce cost

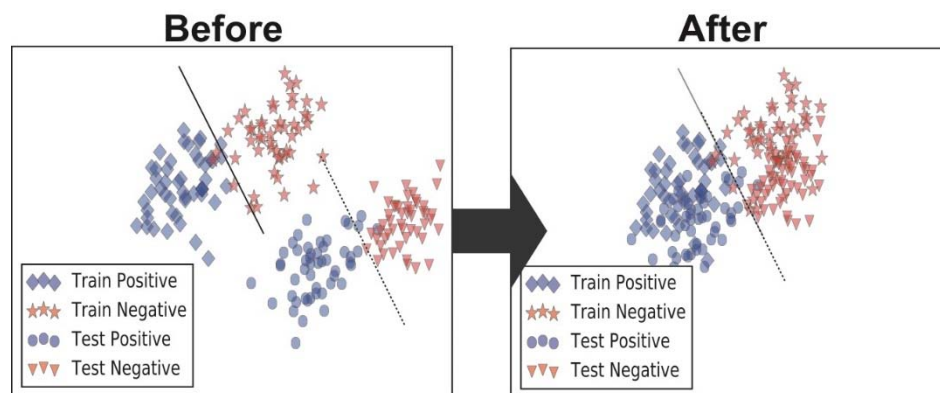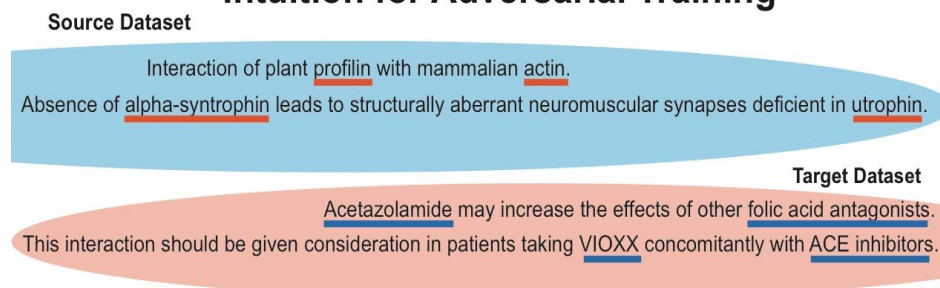- Compelling graphic/visualization
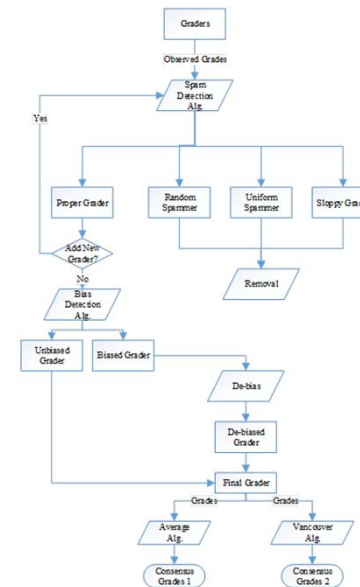
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Adversarial Discriminative Domain Adaptation for Extracting Protein-Protein Interactions from Text

Anthony Rios, Computer Science, University of Kentucky

- Research Category
  - Big Data/Data Mining/Machine Learning

- Relation Extraction
  - Relation extraction is the task of automatically extracting **structured information** from **unstructured documents**.

- Domain Adaptation
  - Domain adaptation is useful when the **source** data distribution is **different (but related)** to the **target** data distribution.
  - We perform **unsupervised domain adaptation**. Meaning, we assume the **target** dataset contains **no labeled instances**.


Intuition for Adversarial Training

Source Dataset

Interaction of plant profilin with mammalian actin.

Absence of alpha-syntrophin leads to structurally aberrant neuromuscular synapses deficient in utrophin.

Target Dataset

Acetazolamide may increase the effects of other folic acid antagonists.

This interaction should be given consideration in patients taking VIOXX concomitantly with ACE inhibitors.

Before — **After**

Train Positive
Train Negative
Test Positive
Test Negative

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Aberrant coordination geometries discovered in the most abundant metalloproteins

Sen Yao, Markey Cancer Center, University of Kentucky

- ## Research Category
  - Big Data & Discovery
    - Structural bioinformatics

- ## Description of Research
  - Compressed angles of metal ions are universal in metalloproteins. They cause complications in structure characterizations, and imply unique functional tendencies.

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PROTEINS

STRUCTURE · FUNCTION · BIOINFORMATICS

WILEY Blackwell
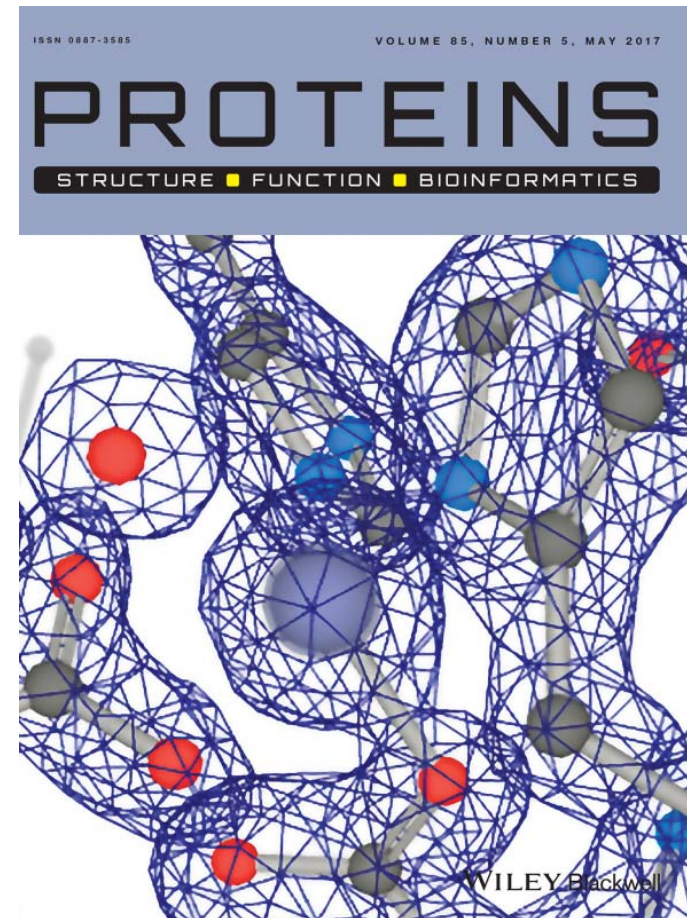
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Distributed Object Segmentation in Big Spatial Data

Hamid Hamraz, Ph.D. Candidate
Department of Computer Science, University of Kentucky

- ## Research Category
  - Big Data/Big Computing
- ## Description of Research
  - Big spatial data is handled as several tiles. Objects may lie across the tile boundaries. This research proposes an efficient way for handling the boundary objects , was implemented and tested for segmenting trees of Robinson Forest in KY.

Tile Map of Robinson Forest

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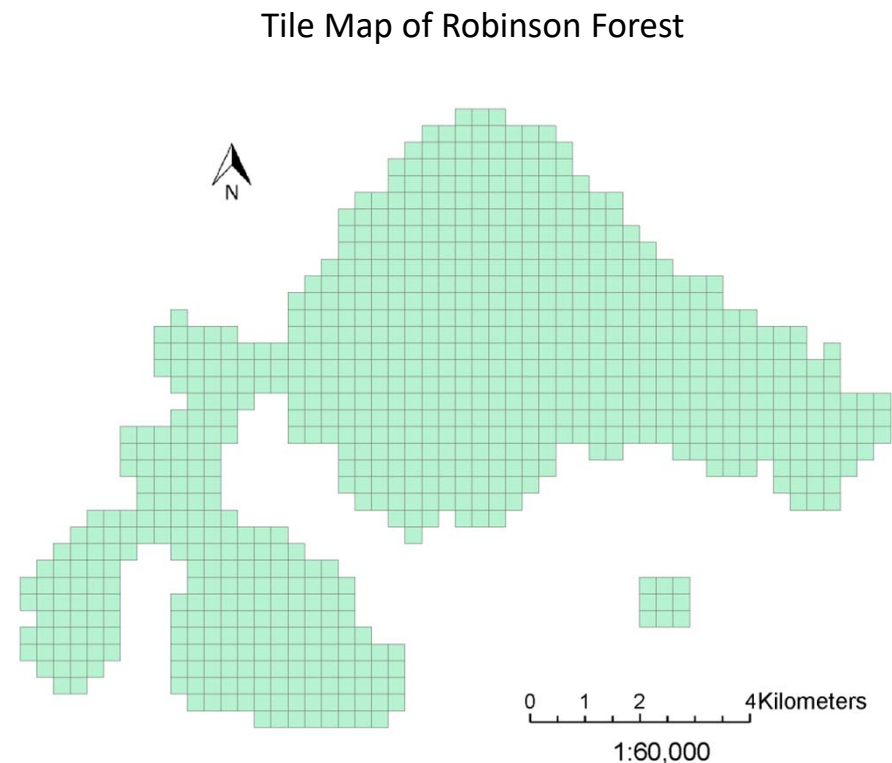
New Explainable Active Learning Framework For Recommender Systems

Sami KHENISSI, University of Louisville
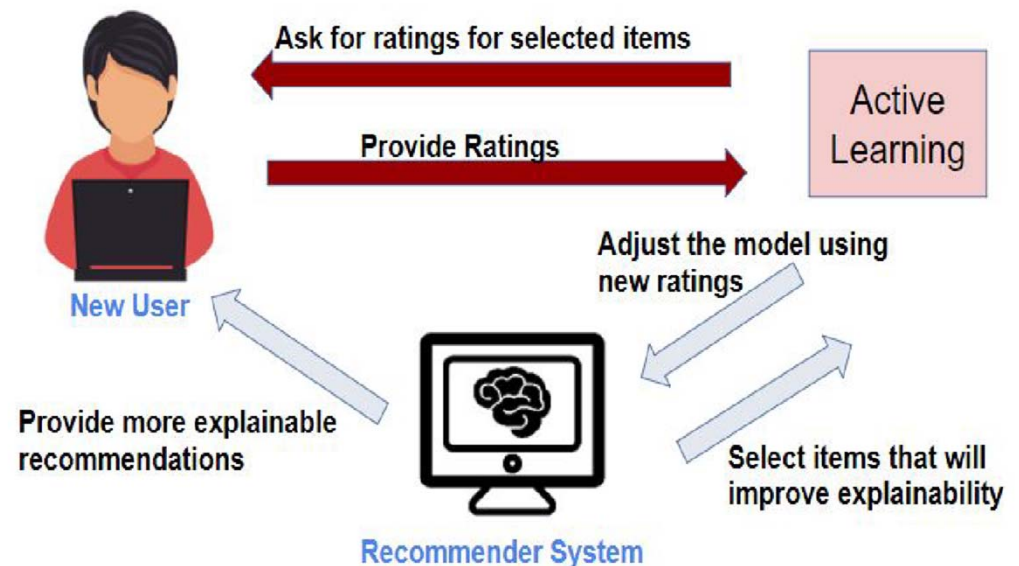## Knowledge Discovery and Web Mining Lab

- **Research Category**
  - Recommender Systems
- **Description of Research**
  - This project will help to increase the explainability of black box Recommender Systems models using a minimum amount of data


Ask for ratings for selected items

Provide Ratings

Active Learning

New User

Adjust the model using new ratings

Provide more explainable recommendations

Select items that will improve explainability

Recommender System

Imputing Trust Network Information in NMF-based Recommendation Systems

Fatemah Alghamedy, Computer Science , University of Kentucky

- ## Research Category
  - ## Recommendation System

- ## Description of Research
  - ## We propose an NMF (Nonnegative Matrix Factorization)-based approach in collaborative filtering based recommendation systems to handle the cold-start users issue, especially for the New-Users who did not rate any items, by utilizing the trust network information to impute missing ratings before NMF is applied.

The Mean Absolute Error MAE before and after impute New-Users

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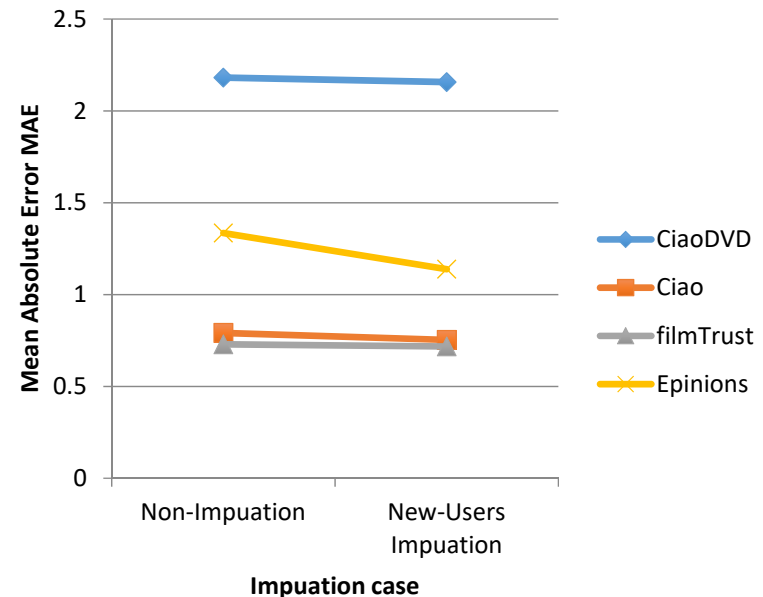
Using Explainability for Constrained Matrix Factorization

Behnoush Abdollahi, Knowledge Discovery & Web Mining Lab, Dept. of Computer Engineering & Computer Science, University of Louisville

- Research Category
  - Big Data, Machine Learning, Recommender Systems
- Description of Research
  - This project presents a novel approach for designing explainable recommender systems that increases transparency while generating accurate results


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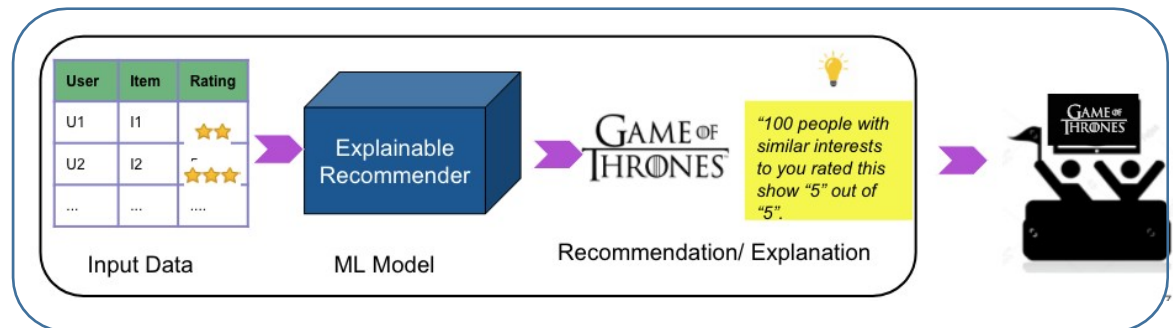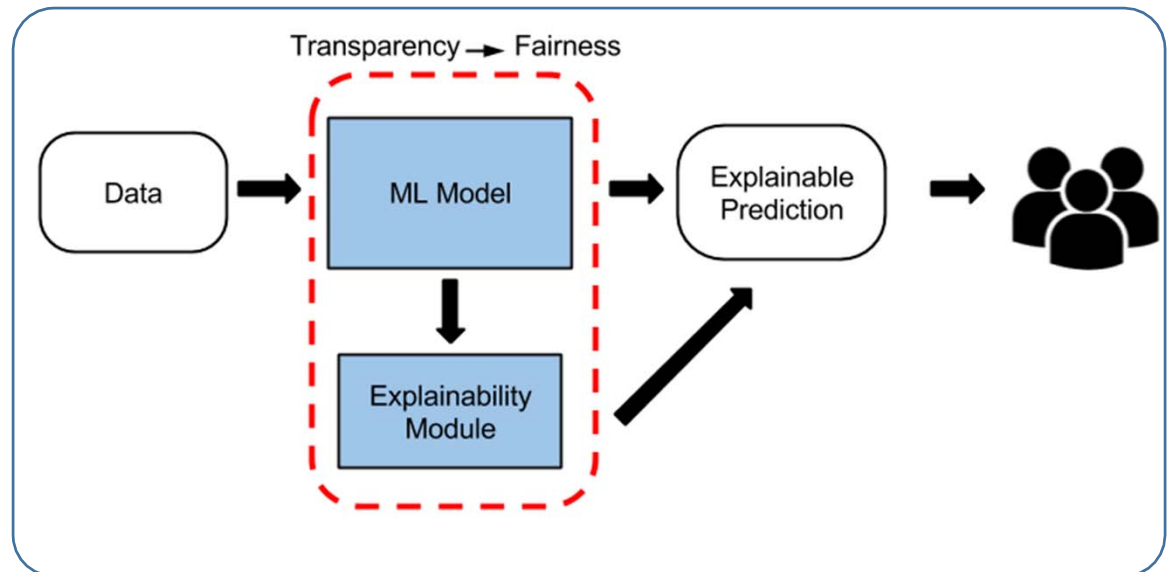
Title: **How Low Can You Go? Feature Selection for Drug Discovery**

Presenter: Derek Jones

Categories: Machine Learning, Bioinformatics

Description: In our work we address the active versus decoy binding interaction prediction task by using a random forest feature selection method to reduce the dimensionality of our feature space. We find that we are able to reduce the dimensionality of our problem by approximately 2 orders of magnitude and achieve comparable performance.
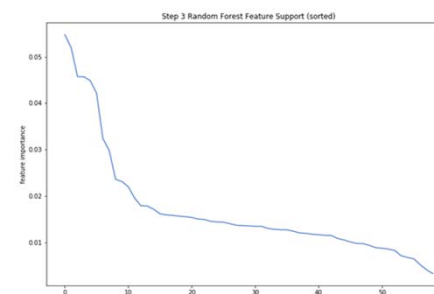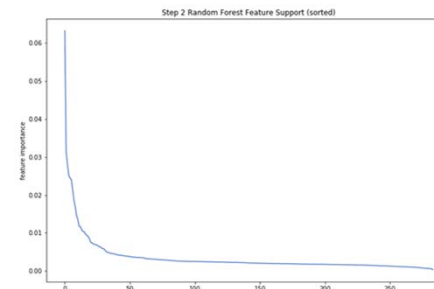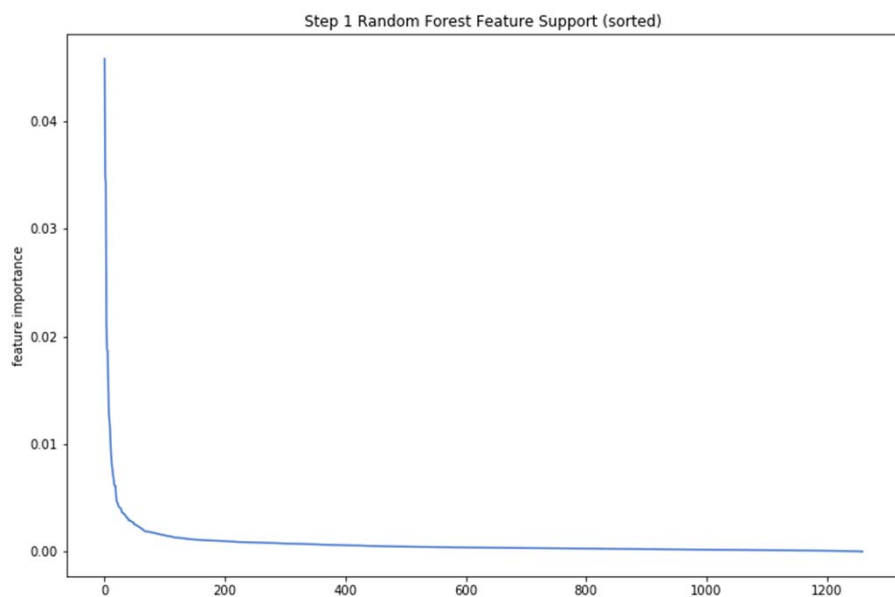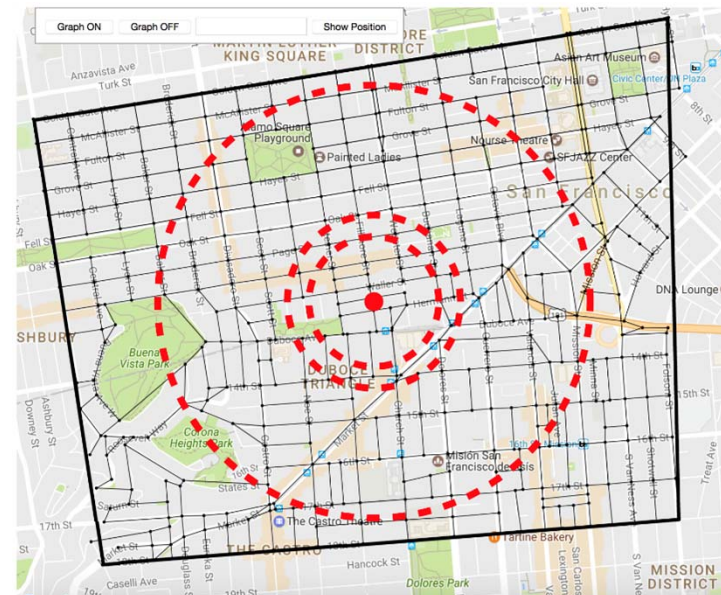
A Network Tomography Approach for Traffic Monitoring in Smart Cities
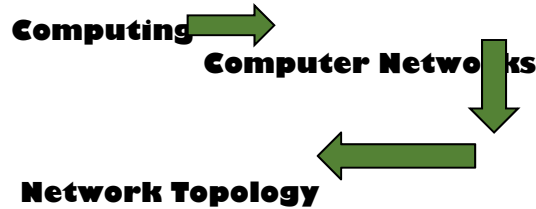
Sara Newman, Ruoxi Zhang
Computer Science, Missouri University of Science and Technology

- ## Research Category
  - ### Network Tomography

- ## Description of Research
  - ### This project involves the formulation of a network tomography approach to traffic monitoring based on the optimization of monitor placement.

- ## Compelling Graphic/Visualization

Bio-Inspired Disaster Response Networks

Vijay K. Shah, Department of Computer Science, University of Kentucky
Advisors: Dr. Simone Silvestri, and Dr. Sajal K. Das (*Missouri S&T, Rolla*)
Collaborator: Satyaki Roy (*Missouri S&T, Rolla*)

CCS²
2017

❖ **Research Category**

Computing

Computer Networks

Network Topology

❖ **Research Description**

This work proposes a *robust and energy-efficient* **disaster response network** *(*DRN), termed **bio-inspired bio-DRN** that mimics the inherent topological robustness of a biological network of living organisms, called *gene regulatory networks* (GRN)

➢ A disaster response network (DRN) is a temporary network constructed by off-the-shelf smart devices for timely information exchange between survivors and responders (in absence of infrastructure communication systems)

Fig. *E.Coli GRN*
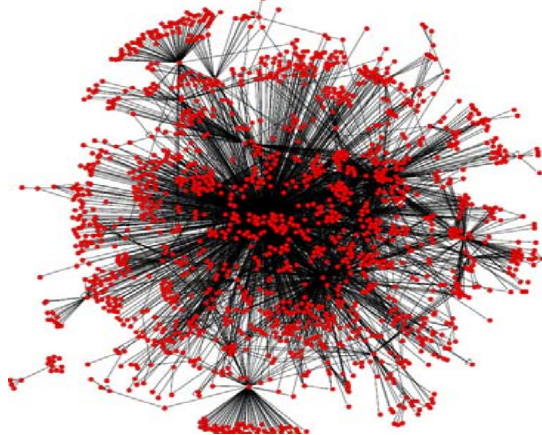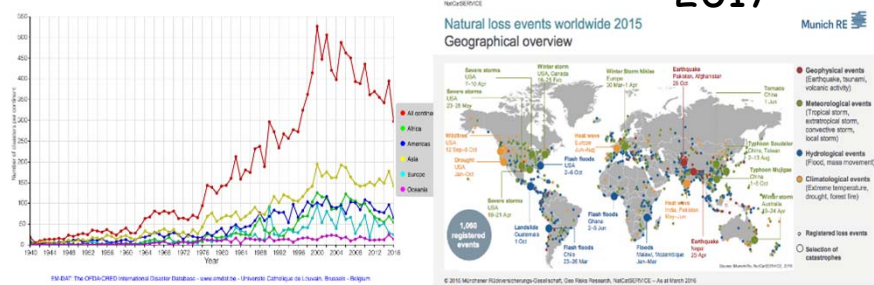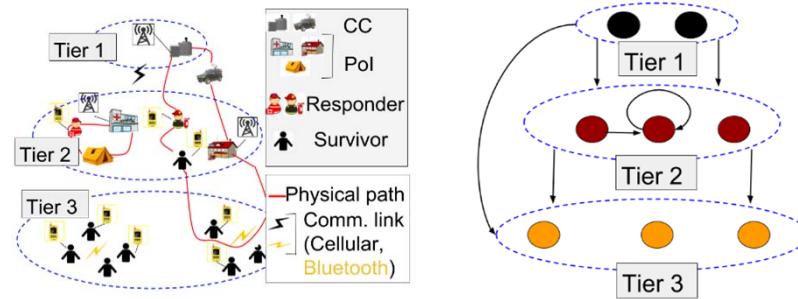

❖ **Network Topology Structure**

Fig. Three tier network topology structure: (a) DRN, and (b) GRN

❖ **Evaluation Results**
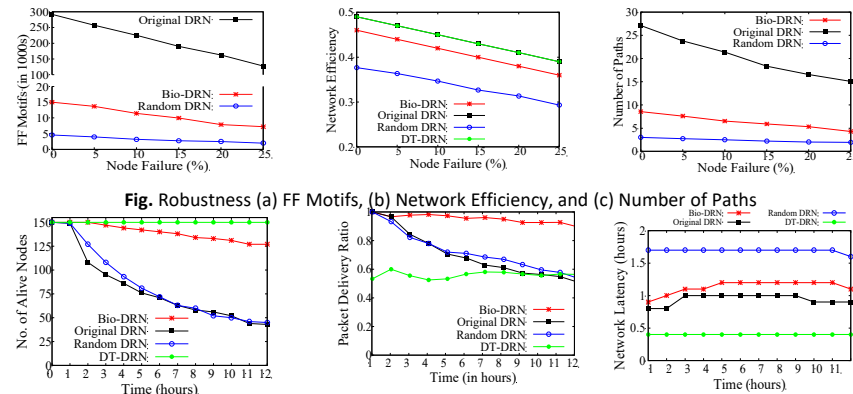

Fig. Robustness (a) FF Motifs, (b) Network Efficiency, and (c) Number of Paths

Fig. (a) Energy Efficiency (b) Packet Delivery Ratio, and (c) Network Latency

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Dynamic Load Balancing based On Live Virtual Machine Migration

Manh Do, Computer Science, Western Kentucky University

- **Research Category**
  - Cloud Computing
- **Description of Research**
  - This project will determine how to dynamic balancing the CPU's usage of all cloud cluster using Live Virtual Machine – KVM feature.

- **After applying Load Balancing Algorithm.**
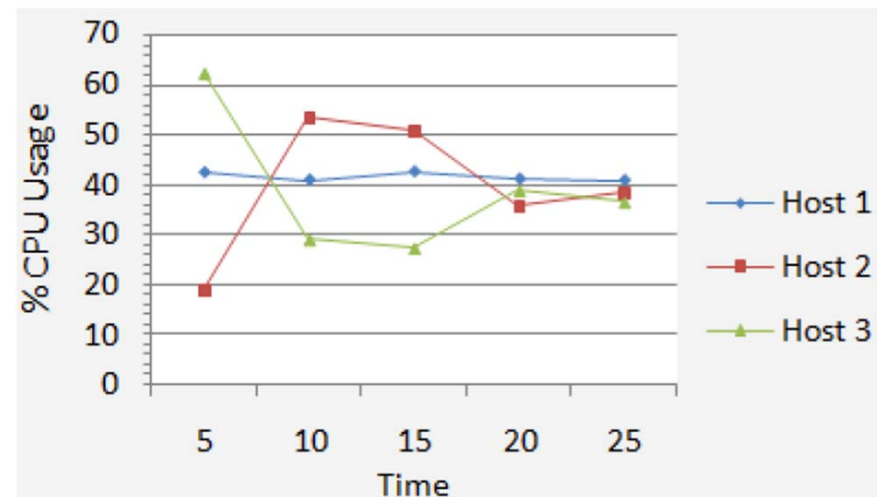
Cloud-Based Text Analytics: Harvesting, Cleaning and Analyzing Corporate Earnings Conference Calls

Michael Chuancai Zhang, Gatton College of Business and Economics, University of Kentucky

- ## Research Category
  - Future Technology (Cloud computing)

- ## Description of Research
  - This project introduces the problems in corporate earnings conference call transcripts harvesting, cleaning, and analyzing processes, and the final solutions to show how we can benefit from modern computation technologies in our research.

- ## Compelling graphic/visualization

Days used for harvesting, cleaning and computing the data

	Manual	Automatic	Manual	Automatic	Local	Cloud
Value	41	15	406	17	270	10
	Harvesting		Cleaning		Computing	