

Research Area: Computational Biology

Modeling of Biological Networks

MISSISSIPPI
EPSCoR Experimental Program to Stimulate Competitive Research

University Participants

Jackson State University (JSU)

Mississippi State University (MSU)

University of Mississippi (OleMiss)

University of Southern Mississippi (USM)



Senior Personnel



Raphael Isokpehi
Hari Cohly
Natarajan Meghanathan



Susan Bridges
Bindu Nanduri
Changhe Yuan
Andy Perkins
Shane Burgess
Mahalingam Ramkumar
Yoginder Dandass



Chaoyang Zhang
Nan Wang
Preetam Ghosh
Frank Moore
Robert Diehl
Jonathan Sun

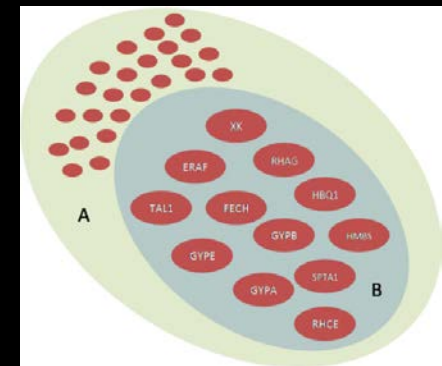
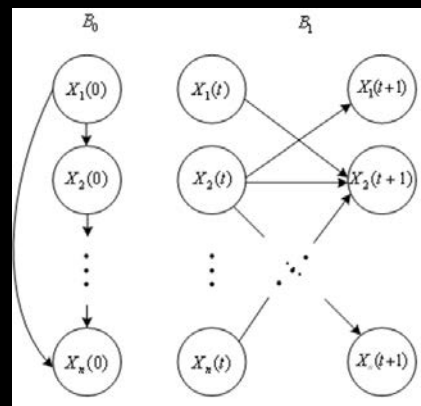
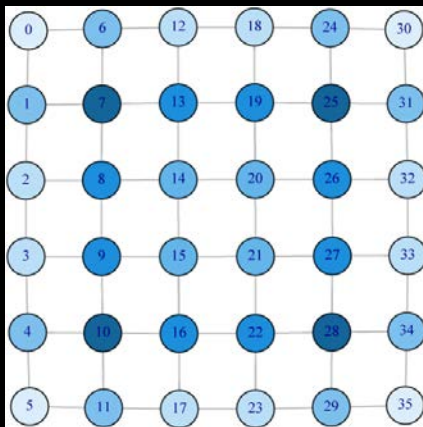


Dawn Wilkins
Yixin Chen

Comp Bio Cluster Long-Term Goals



1. Develop nationally recognized and respected multi-institutional programs of excellence in **modeling of biologically relevant complex systems**.
2. Develop national expertise in **modeling of biological networks**.
3. Develop **cyber-enabled** data mining, data integration, data tracking, and model learning algorithms **for building models of biological networks**.



Goals of Current EPSCoR Award



1. Integrate research in **modeling and simulation of biologically complex systems** to make significant contributions within the areas of **multi-scale simulation of biological systems** (BioSim), **modeling of biological networks** (CompBio) and **modeling and simulation of nanoscale chemistry** (CompChem).
2. Foster program and discipline **integration and synergy across research focus areas**, across universities, and internationally to strengthen the statewide impact of EPSCoR funded initiatives and to develop new **cross-cutting research**.
3. Increase the number of people from **underrepresented groups** at all levels – undergraduate, graduate, postdoc, and faculty – participating in **modeling and simulation** within the EPSCoR jurisdiction.

Goals of Current EPSCoR Award

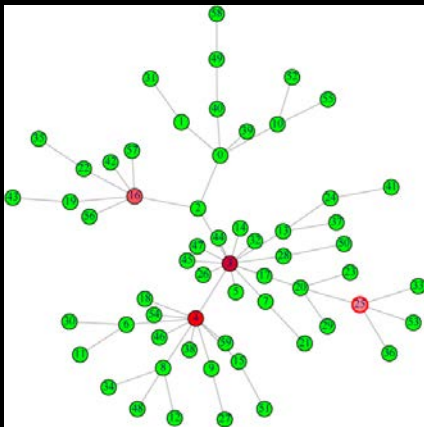


4. **Increase the workforce** in the computational sciences, particularly in computational biology, computational chemistry, and computational biosimulation, by bringing together researchers, teachers, entrepreneurs, and industries in **collaborative partnerships** to build regional competitiveness.
5. Develop an **integrated, virtual community** of competitive research teams to address large **multidisciplinary research areas** by enhancing connectivity and interaction through **cyberinfrastructure**.
6. **Broaden** the understanding, reach and impact of **STEM** among students, policy makers, industrial leadership, and the general public.

Research Activities (RA) within the Comp Bio Cluster

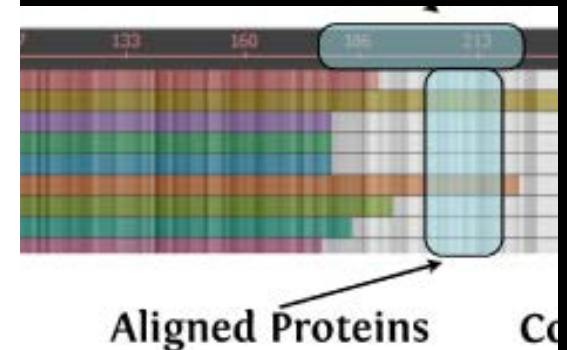


1. Graph-based algorithms to integrate transcript and protein data
2. Binary data models of complex biological data sets
3. New algorithms for building explainable models of biological networks
4. Data provenance methods for managing data sources used to build biological networks



Algorithm 1 KSD Algorithm

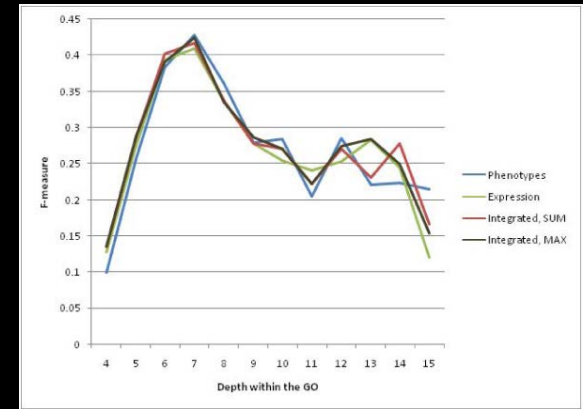
```
1 Get the Laplacian  $\mathcal{L}$  of the input graph  $G$ 
2 Choose and compute the kernel matrix  $K$ 
3 FOR (every vertex  $m$  in  $G$ )
4   FOR (every vertex  $i$  in  $G$ )
5      $t = \sqrt{K_{mm} + K_{ii} - 2K_{mi}}$ 
6     IF  $t = 0$ 
```



RA-1: Develop Graph-based Algorithms to Integrate Transcript and Protein Data



1. A graph-theoretic approach to determine unique signature relationships between the biological pathways and the genomic information of different species belonging to a genera of microbial pathogens (JSU)
2. Integrating transcriptomic and proteomic data sets based upon Gene Ontology (GO) term similarity (MSU)
3. Analysis of high throughput Solexa transcriptomic data (MSU)
4. Bacterial repeat analysis (MSU)

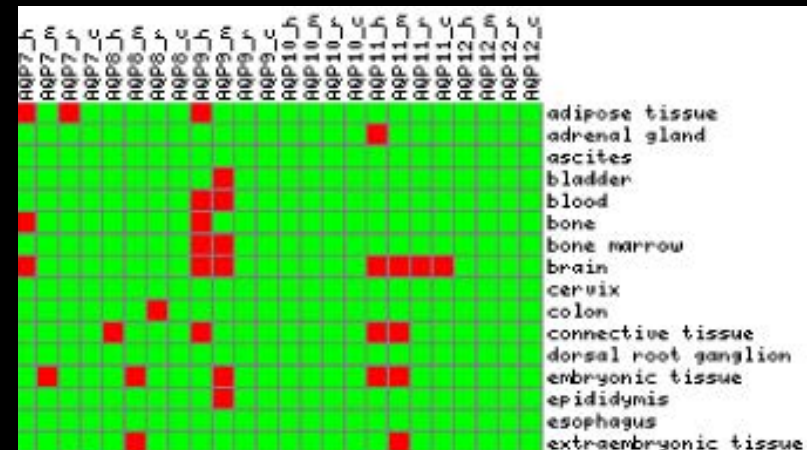


RA-2: Develop Binary Models of Complex Datasets



1. A quadrant-based binary data model for assessing the functional state of human organ systems (JSU)
2. Binary Models of Gene Networks (JSU, MSU)

Organs/Organ systems	F0	F1	Organs/Organ systems	F0	F1
Right eye			Cardiovascular system		
Right ear, Nose, Maxillary sinus			Cerebral zone (vessels)		
Jaw, Teeth right side			Abdominal zone		
Throat, Larynx, Trachea, Thyroid gland			Hypophysis		
Jaw, Teeth left side			Thyroid gland		
Left ear, Nose, Maxillary sinus			Pancreas		
Left eye			Adrenal		
Cerebral zone (cortex)			Urino-genital system		
Thorax zone			Spleen		
Lumbar zone			Nervous system		
Coccyx, Pelvis minor zone			Epiphysis		
Blind gut			Duodenum		
Appendix			Ileum		
Ascending colon			Mammary glands, Respiratory system		
Transverse colon			Jejunum		
Descending colon			Right part of heart		
Thorax zone, Respiratory system			Activation coefficient		
Immune system			Integral area		
Gallbladder			RMS of Integral area		
Liver					



RA-3: Develop New Algorithms for Building Explainable Models of Biological Networks

1. Learning and explaining gene interaction networks (MSU)
2. Identifying interspecies interactions in non-model organisms (MSU)
3. Diffusion kernel large margin random forests classification for integrated biological prediction (OleMiss)
4. Probabilistic minimum description length principle on information theoretic approaches for reconstructing gene regulatory networks (USM)

RA-4: Develop Data Provenance Methods for Managing Data Sources used to Build Biological Networks



1. Comparison of a Graph database and a Relational database :
A data provenance perspective (OleMiss)
2. Learning to rank using 1-norm regularization and convex hull reduction (OleMiss)
3. An empirical comparison of data management methods (OleMiss)
4. An algorithm to self-extract secondary keywords and their combinations based on abstracts collected using primary keywords from online digital libraries (JSU)

Discipline Integration and Synergy across Research Focus Areas, across MS-EPSCoR Universities



CompChem

CompBio

BioSim

CompBio

BioSim



CompChem

CompChem



CompBio

BioSim

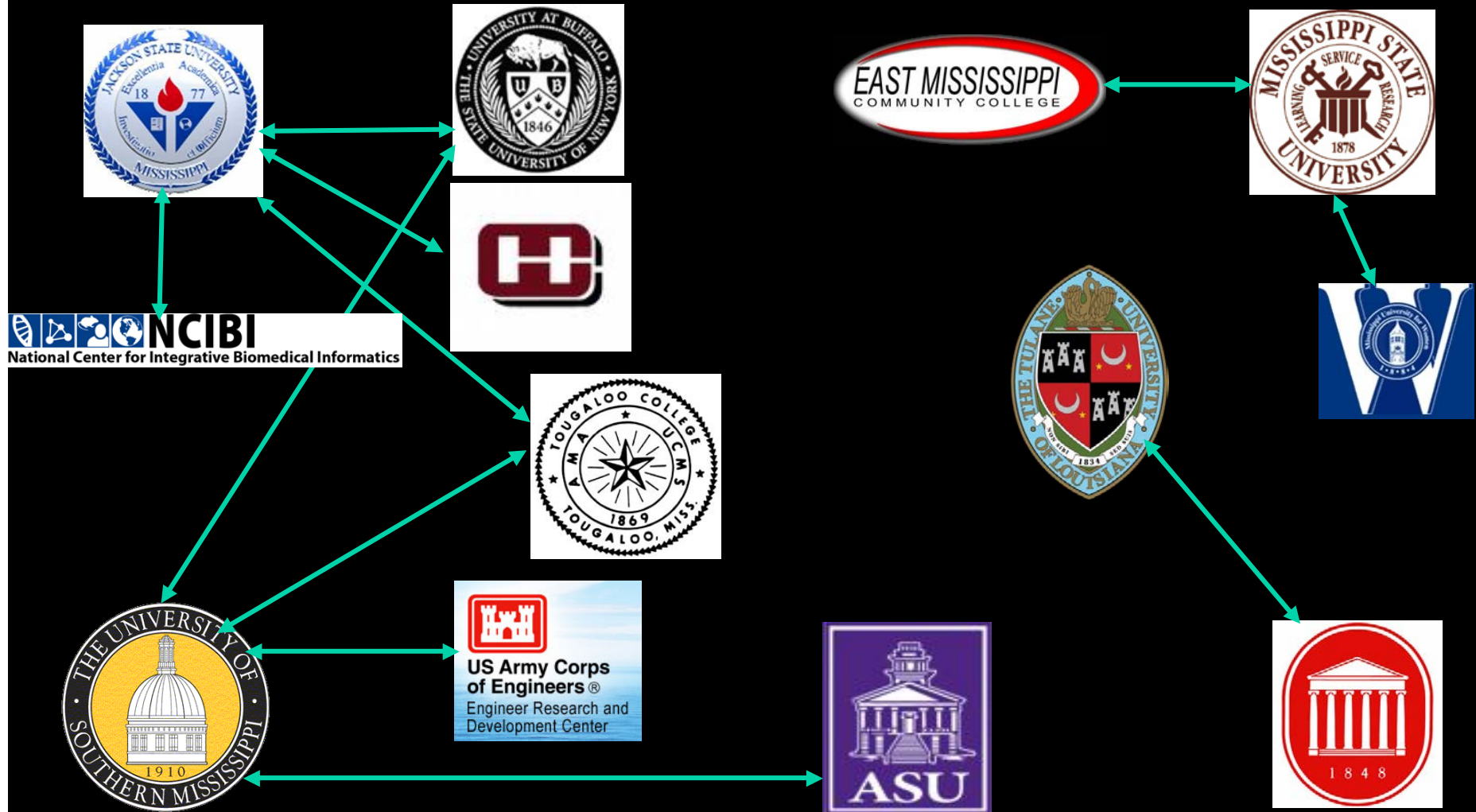
CompBio

BioSim

CompChem



Collaborations of the Comp Bio Cluster with other Universities/ Colleges/ Research Centers



Proposals Funded for 2009-2010

MS-EPSCoR Comp Bio Faculty (Listed by Agencies)



➡ \$963,949 (9 Proposals)



➡ \$541,333 (5 Proposals)



➡ \$408,619 (3 Proposals)



➡ \$67,208 (2 Proposals)



➡ \$20,000 (1 Proposal)



➡ \$15,000 (1 Proposal)

Proposals Submitted for 2009-2010 MS-EPSCoR Comp Bio Faculty (Listed by Agencies)



—————▶ **\$7, 902,155 (12 Proposals)**



▶ **\$1, 573,799 (4 Proposals)**



—————▶ **\$1, 200,000 (2 Proposals)**



▶ **\$750,000 (1 Proposal)**



▶ **\$124,295 (1 Proposal)**



—————▶ **\$20,000 (1 Proposal)**



Summary of Research Accomplishments (2009-2010)

1. Proposals funded – ongoing or newly approved (21): \$2M
2. Proposals submitted – pending or denied (21): \$11.5M
3. Peer-reviewed Journal papers published or accepted: 13
4. Book Chapters published or accepted: 3
5. Peer-reviewed Conference papers published or accepted: 9
6. Abstracts/ Oral Presentations: 13
7. Poster Presentations: 18
8. Journal articles under peer-review: 8
9. Conference articles under peer-review: 7
10. Number of courses taught: 4 graduate courses
11. Number of students funded and/or advised: 19 graduate and 10 undergraduate students

MS EPSCoR Comp Bio Faculty Publication Network



HC

NM

DW

YC



RI

SMB

PG

RD

CZ

BN

JS

NW

AP



CY

SCB

YD

MR



Education, Outreach Activities and Professional Services of Comp Bio Faculty (2009-2010)



1. Recruit students from the community colleges for the REU program in Computational Biology at MSU
2. JSU faculty and students offered workshops to Elementary, Middle and High School students on the Overview of Bioinformatics (part of NASA Educator Resource Workshop) and on Investigating Bacteria as a Scientist
3. Several EPSCoR faculty served in the TPC of several international conferences in the areas of Bioinformatics, Computational Biology, Systems Biology and other relevant fields
4. Several EPSCoR faculty also served in the editorial board and/or as reviewers of journals in the areas of Bioinformatics, Computational Biology, Systems Biology and other relevant fields

Jackson State University
Center for Bioinformatics & Computational Biology
College of Science, Engineering & Technology

Bioinformatics Awareness Month 2010

The key activities of the Month include:

- ✓ **Bioinformatics Open House**
- ✓ **Lectures and Computer Laboratory Sessions on Bioinformatics Topics**
- ✓ **Guest Lectures**
- ✓ **Technology and Informatics Luncheon**
- ✓ **Speed Networking**

Our collaborators from Pittsburgh Supercomputing Center at Carnegie Mellon University, Mississippi Computational Biology Consortium, Arkansas State University, Meharry Medical College, Virginia Bioinformatics Institute, University of Florida, Mississippi State University and University of Michigan will be visiting Jackson State University starting from April 7, 2010.

For Complete Schedule Visit Us At
<http://compbio.jsums.edu/awareness2010>

For More Information Call 601-979-0328
Just Science Hall 117c

Date/Time	Event	Location
April 7 12p.m.-1p.m.	Bioinformatics Awareness Month Kick-Off and Open House	Lecture Room 148 JSH
April 7 1p.m.-4p.m.	Poster Session/ Open House / Student Workshop Registration	Research Lab 117 C JSH
April 8 10a.m.-11a.m.	NBACC	Research Lab 117 C JSH
April 8 11a.m.- 6p.m.	National Laboratory Mock Interviews	Conference Room 250 JSH
Click Here for Dates	Workshop Series: What is Bioinformatics? \$200 Stipend upon completion	Research Lab 117 C JSH
April 14 2p.m.- 3p.m.	Genomics of Vibrio Foodborne Pathogens	Lecture Room 148 JSH
April 15 8a.m.- 5p.m.	Mississippi EPSCOR Annual Meeting	MS E-Center



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RESEARCH HIGHLIGHTS

Gene Regulatory Networks – CBBL USM



1. Research Activities

1. Develop data analysis and preprocessing pipeline
2. Develop new models (State-space model and stochastic model)
3. Improve inference approaches (information theory, probabilistic Boolean model, dynamic Bayesian networks)
4. Develop new Bayesian learning and optimization approaches



2. Proposals (submitted to NSF, ORNL, DOE and US Army)

3. Research Group (four faculty members, 7 PhD students, two visiting scholars and another one plans to join CBBL, Peng Li (2009) is a NIH postdoc)

4. Research Collaboration

1. Established a long-term Research Collaboration with ERDC, US Army
2. with Shanghai Institutes for Biological Sciences (SIBS), Chinese Academy of Sciences

5. Ongoing Research Related to Bio-Cyberinfrastructure

1. Developing knowledgebase for earthworm toxicogenomics
2. Developing biological networks analysis and reconstruction server

Gene Regulatory Networks – CBBL USM



1. Integrate Research and Education

1. Offered two new graduate courses (Computational Biology, Modeling Biological Networks)
2. Two visiting scholars and another one plan to join CBBL this summer.
3. Weekly group meeting
4. International Exchange Program (Nan Wang)
5. MCBIOS 2010: received best student poster award



2. Participated in **Dialogue for Reverse Engineering Assessments and Methods (DREAM) Challenge Competition** at RECOMB conference in 2008 and 2009.

1. CBBL USM team won the second place

3. Research Services

1. Joe Zhang, Co-Founder and Program Chair of The 2009 International Joint Conferences on Bioinformatics, System Biology and Intelligent Computing (IJCBS 09) , Shanghai, China, August 3-5, 2009 (<http://www.isibm.org/IJCBS>).
2. Joe Zhang, Steering Committee Co-Chair at The ACM 2010 International Conference on Bioinformatics and Computing Biology (ACM-BCB 2010) , Buffalo, NY, Aug 2-4, 2010.
3. Preetam Ghosh, Associate Bioinformatics Director of NIH-MFGN



Bioinformatics Tools Categorizer

Version 1.0

A resource for searching categories of tools published in *Bionformatics*



Year	Category	Search with Keyword
<input type="text"/>	<input type="text"/>	<input type="text" value="regul"/>
<input type="button" value="Submit"/>	<input type="button" value="Reset"/>	<input type="checkbox"/>

Results:...

Search characteristics: Search term is = 'regul'

55 Articles found.

7 Links that are decayed or null.

12.73% Decayed Links.

- ☐ Links are available
- ☐ Links are unavailable

No. Title of Article in Bioinformatics

- 1 [Combining statistical alignment and phylogenetic footprinting to detect regulatory elements](#)
- 2 [A system for generating transcription regulatory networks with combinatorial control of transcription](#)
- 3 [Fast network component analysis \(FastNCA\) for gene regulatory network reconstruction from microarray data](#)
- 4 [Implementation of a regulatory gene network to simulate the TH1/2 differentiation in an agent-based model of hypersensitivity reactions](#)
- 5 [Discovering regulatory motifs in the *Plasmodium* genome using comparative genomics](#)
- 6 [Synchronous versus asynchronous modeling of gene regulatory networks](#)

Category

- ☐ SEQUENCE ANALYSIS
- ☐ SYSTEMS BIOLOGY
- ☐ GENE EXPRESSION
- ☐ SYSTEMS BIOLOGY
- ☐ GENOME ANALYSIS
- ☐ SYSTEMS BIOLOGY

- 50 [GAME: detecting *cis*-regulatory elements using a genetic algorithm](#)
- 51 [Inferring gene regulatory networks from multiple microarray datasets](#)
- 52 [Adding sequence context to a Markov background model improves the identification of regulatory elements](#)
- 53 [A regularized discriminative model for the prediction of protein-peptide interactions](#)
- 54 [Short fuzzy tandem repeats in genomic sequences, identification, and possible role in regulation of gene expression](#)
- 55 [A novel algorithm for detecting differentially regulated paths based on gene set enrichment analysis](#)

- ☐ SEQUENCE ANALYSIS
- ☐ GENE EXPRESSION
- ☐ SEQUENCE ANALYSIS
- ☐ SEQUENCE ANALYSIS
- ☐ GENOME ANALYSIS
- ☐ GENE EXPRESSION

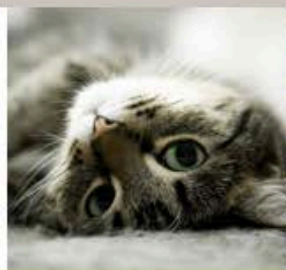
AgBase

[Version: 2.00]

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“AgBase is a curated, open-source, web-accessible resource for functional analysis of agricultural plant and animal gene products.”



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[Bovine Gene Atlas](#)

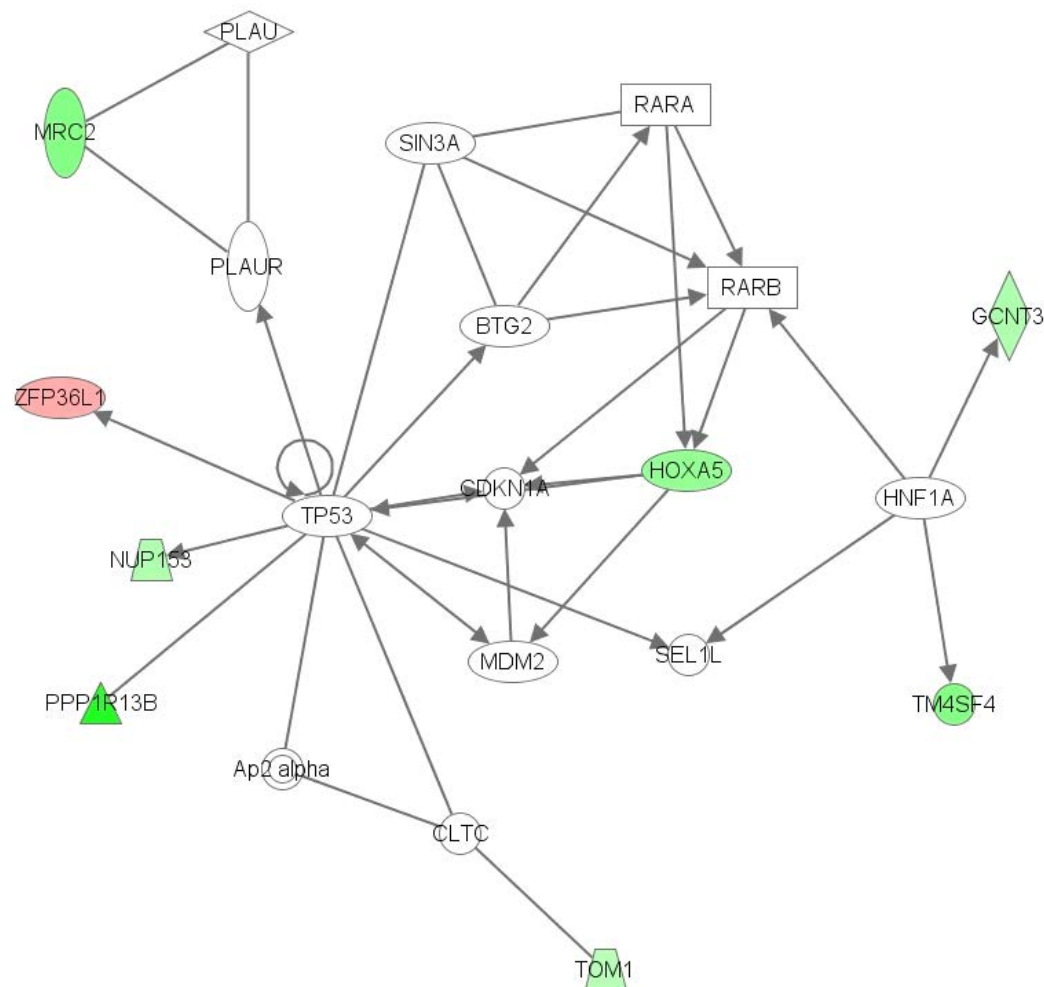


[Array Annotation](#)



[Structural vs. Functional
Annotation](#)

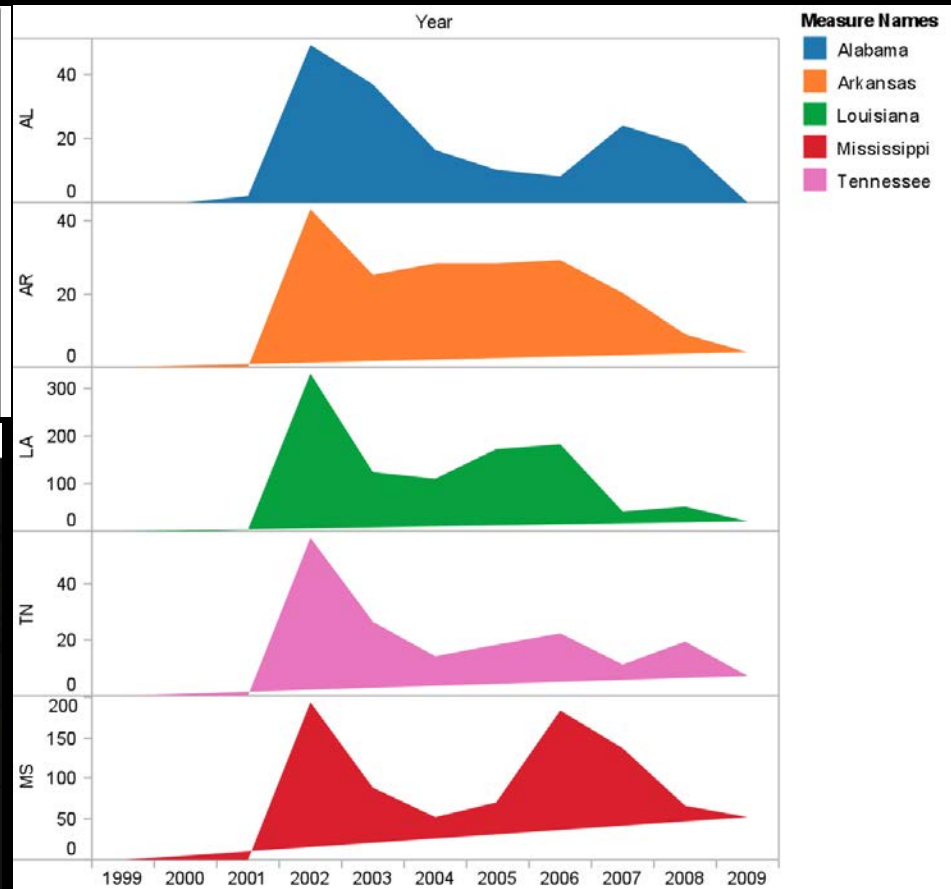
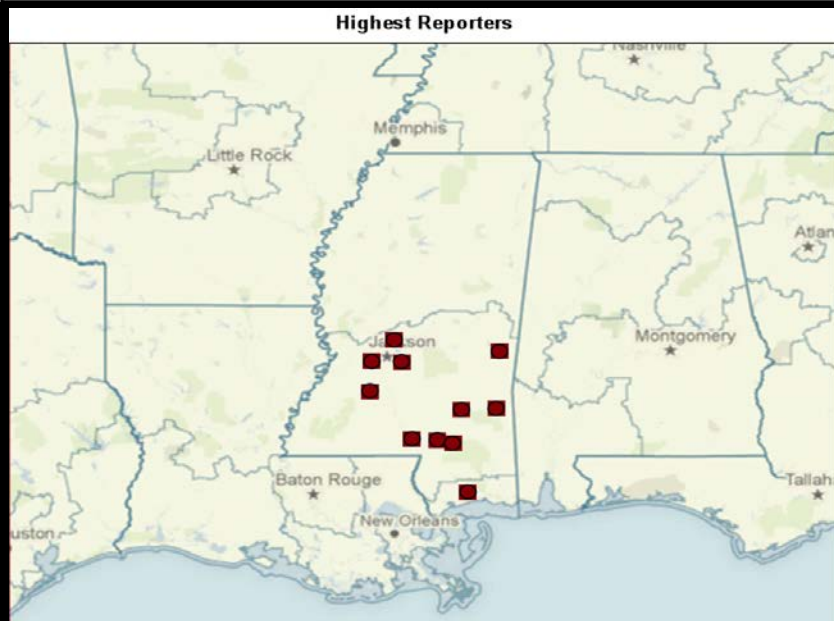
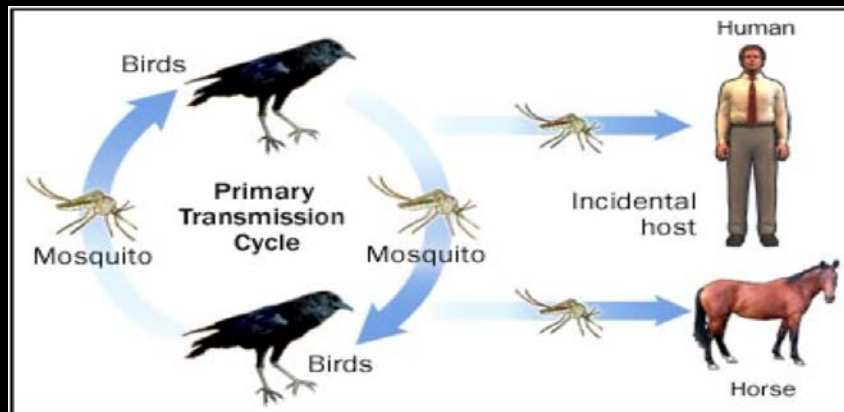
Gene Network of Keratinocytes in Response to Chronic Arsenic



Expression Data Generated at JSU
Cohly, Isokpehi, Graham, Udensi

Pathway Data Analyzed at MSU
Nanduri, Bridges

West Nile Virus Ecology in Mississippi – Public and Animal Health Threat



Human West Nile Virus Infection – Trends in Mississippi and Neighboring States
Gabrielle A. Cooper, Oluwakemi O. Oluwatuyi, Sean R. Scott, Tolulola O. Oyeleye,
Matthew O. Anyanwu, Hari H.P. Cohly, and Raphael D. Isokpehi

What are the SpatioTemporal Models that has been used to Study West Nile Virus Transmission Dynamics? – Text Mining



WEST NILE - West Nile Virus Sentence Database

Database of Sentences Derived from PubMed Citations linked to West Nile Virus

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<http://compbio.jsums.edu/wnv>

WEST NILE: West Nile Virus Sentence Database

Collection of datasets of sentences derived from PubMed Abstracts on West Nile Virus

The search Keyword/PMID is **spati**

JSU Student to Visit Robb Diehl at USM to learn about Bird Migration Patterns in Mississippi

#	Sentence Identifier (sort)	Sentence Text	PMID (sort)
1	16806542_4	Kulldorff's scan statistic was used to identify spatial-temporal clusters in both the human and horse cases.	16806542
2	16935481_1	Spatiotemporal reasoning about epidemiological data.	16935481
3	16935481_2	OBJECTIVE: In this article, we propose new methods to visualize and reason about spatiotemporal epidemiological data.	16935481
4	16935481_3	BACKGROUND: Efficient computerized reasoning about epidemics is important to public health and national security, but it is a difficult task because epidemiological data are usually spatiotemporal, recursive, and fast changing hence hard to handle in trad	16935481
5	16935481_6	In the system, users can do many interesting reasonings based on the spatiotemporal dataset and the recursively defined risk evaluation function through the SQL query interfaces.	16935481
6	16935481_9	Our general solution for reasoning about epidemics and related spatiotemporal phenomena enables one to solve many problems similar to WNV without much modification.	16935481
7	17507930_7	We demonstrate significant changes in population trajectories for seven species from four families that concur with a priori predictions and the spatio-temporal intensity of pathogen transmission.	17507930
8	19440960_2	In this research, community level spatial models were developed for determining mosquito abundance and environmental factors that could aid in the risk prediction of West Nile virus (WNV) outbreaks.	19440960
9	19440960_3	Adult Culex pipiens and Culex restuans mosquitoes and multiple habitat covariates were collected from nine sites within Cook County, Illinois, USA, to provide spatio-temporal information on the abundance of WNV vectors from 2002 to 2005.	19440960
10	19440960_9	Spatial dependence of the covariates of Cx. restuans and Cx. pipiens oviposition sites were indexed using semivariograms, which suggested that all main effects of the explanatory variables were statistically significant in the model.	19440960
11	16989568_1	Modeling the spatial distribution of mosquito vectors for West Nile virus in Connecticut, USA.	16989568

MCBIOS 2010

February 18-19 at Arkansas State University



1. Dawn Wilkins (OleMiss)
 - Past President, Managed Judging of Student Oral Presentations
2. Susan Bridges (MSU)
 - Elected President-Elect for 2011
3. Raphael Isokpehi (JSU)
 - Board Member and Networking Chair for MCBIOS 2010 Meeting
4. Andy Perkins (MSU)
 - Chair, Poster Session

MCBIOS.ORG

MIDSOUTH COMPUTATIONAL BIOLOGY & BIOINFORMATICS SOCIETY

MCBIOS 2010

February 18-19 at Arkansas State University



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[MCBIOS V \(2008\)](#)

[MCBIOS VI \(2009\)](#)

[MCBIOS VII \(2010\)](#)

MCBIOS 2010 Awards

Congratulations to the 2010 student award winners!

Oral Presentations

First Place:

Heidi Pagan, Mississippi State University (MSU)

"Lineage Specific Activity from Novel Piggyac Elements and Evidence of Horizontal Transfer in Mouse Lemurs (*Microcebus*)" Mentor: Dr. David Ray



Second place:

Juliet Tang, Mississippi State University (MSU)

"Assembling a Novel Fungal Genome from Short Read Sequencing Data"

Mentor: Dr. Susan Diehl



Third place:

Aleksandra Markovets, Mississippi Valley State University (MVSU)

"Promoter Prediction in *Halothiobacillus Neapolitanus* C2 based on stress-induced DNA duplex destabilization"

Mentors: Dr. Abigail Newsome and Dr. Charles Bland



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Poster Presentations

Biological Focus

First place:

Neal Platt, Mississippi State University
"Recognition, Categorization, and Characterization of Transposable Elements in a Non-muroid Rodent: *Spermophilus tridecemlineatus*"

Mentor: Dr. David Ray

Second place:

Gabrielle Cooper, Jackson State University
"West Nile Virus Infection in Humans: Trends from 2003-2008 in Mississippi and its Neighboring States"

Mentors: Dr. Raphael Isokpehi and Dr. Hari Cohly

Third place:

Mais Ammari, Mississippi State University
"Computational Analysis of Bovine Viral Diarrhea Virus Infected Monocytes: Identification of Cytopathic and Non-Cytopathic Strain Differences."

Mentor: Dr. Lesya Pinchuk

Computational Focus

First place:

Vijender Chaitankar, University of Southern Mississippi
"Transcriptional time lagged information approach to improving the accuracy of gene regulatory network reconstruction"

Mentor: Dr. Chaoyang Zhang

Second place:

Lakshmi Pillai, Mississippi State University
"GORIF: A Tool for Generifs to Gene Ontology"

Mentor: Dr. Shane Burgess

Third place:

Christy Gearheart, University of Louisville
"Design of a DNA-Based Shift Register"



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MidSouth COMPUTATIONAL BIOLOGY & BIOINFORMATICS SOCIETY

MCBIOS 2010

February 18-19 at Arkansas State University



Mississippi Participants at MCBIOS 2010

