

*Connecting people and resources to  
accelerate discovery by empowering the  
science gateway community*



# Science Gateways Summer 2017 Interns



Award  
Number  
ACI-1547611

**Jacob Harless**  
**College of William & Mary**  
**Mentor: Drew LeMar**



My name is Jacob Harless and I am a rising senior computer science major at the College of William and Mary in Williamsburg, VA.

I worked with Dr. LaMar at William and Mary as a web developer on the QUBESHub.org website. I worked on adding components and plugins to the site, which used the HubZero Content Management System, itself based on Joomla!. I performed backend development in PHP and some frontend work with HTML, CSS, and Javascript.

**Joel Gonzalez-Santiago**  
**Purdue University**  
**Mentor: Lynn Zentner**



My name is Joel Gonzalez-Santiago and I worked this summer to identify ways for nanoHUB to be self-sustaining. The nanoHUB website is a National Science Foundation funded nonprofit that engages the nano community. It is the largest resource hub for nanotechnologies.

Nonprofits like nanoHUB are tasked with finding financial sustainability after the grants end.

**Hagen Hodgkins**  
**Purdue University**  
**Mentors: Joseph Yun**  
**Kevin Wojkovich**



The goal of this project was to create a proof-of-concept science gateway for the acquisition, storage, sharing, analysis, and visualization of social media data, named the Social Media Macroscope. This program will provide an innovative, easy-to-use, and powerful science gateway for research utilizing social media data. It will make utilizing social media data with data science approaches more accessible to researchers and provide a collaborative platform for researchers from various .

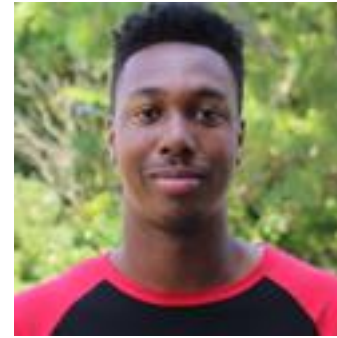
**Tatyana Matthews, TACC**  
**Mentor: Dr. Ritu Arora,**  
**Texas Advanced Computing Center**



Tatyana Matthews worked this summer on an Interactive Parallelization Tool (IPT). IPT will help scientists, engineers, and students build on their customary use of C/C++/Fortran to create more efficient programs that can run on advanced HPC platforms. IPT will be made available to the community as open-source code, and also through a web-portal for convenient code generation and testing on computational resources of the national cyberinfrastructure (CI).

# Disaiah Bennett Thomas Johnson III Indiana University

Both Disaiah and Thomas received the SGCI academic year scholarship and were selected by the SROC program at IU. Interns toured the IU SGCI offices to meet staff and were introduced to the BigRed facilities.



**Mentors**  
**XiaoFeng Wang, Apu Kapadia**

# Science Gateways 3-day Computational Chemistry Workshop @ Jackson State University

## UNIVERSITIES REPRESENTED

Auburn University

University of Houston

Louisiana State University

Spelman College

Binghamton University

Jackson State University

North Carolina A&T State University

University of California

## HOSTED BY

\*Science Gateways Community Institute (SGCI)

\*Jackson State University (Interdisciplinary Nanotoxicity Center)

\*Molecular Sciences Software Institute (MoSSI)

# 3-day Computational Chemistry Workshop at Jackson State University



Professor Vince Ortiz is shown with Auburn PhD student



Dr. Sudhakar V. Pamidighantam



# WORKSHOPS

- Apache Airavata Science Gateway Framework •Computational •Chemistry: New Approaches
- Extension to SEAGrid: Application
- GUI's, Jupyter
- Introduction to Science Gateways Community
- MoISSI Vision MoISSI - Student Requirements/Gateways
- NSF - Vision NSF Chemistry Programs
- Orbital Concepts
- SEAGrid - Deploying Resources/Applications
- SEAGrid - Web/Desktop Portals
- SEAGrid - Hands On Sessions
- SEAGrid - Science Exemplars
- SEAGrid - Undergraduate Research

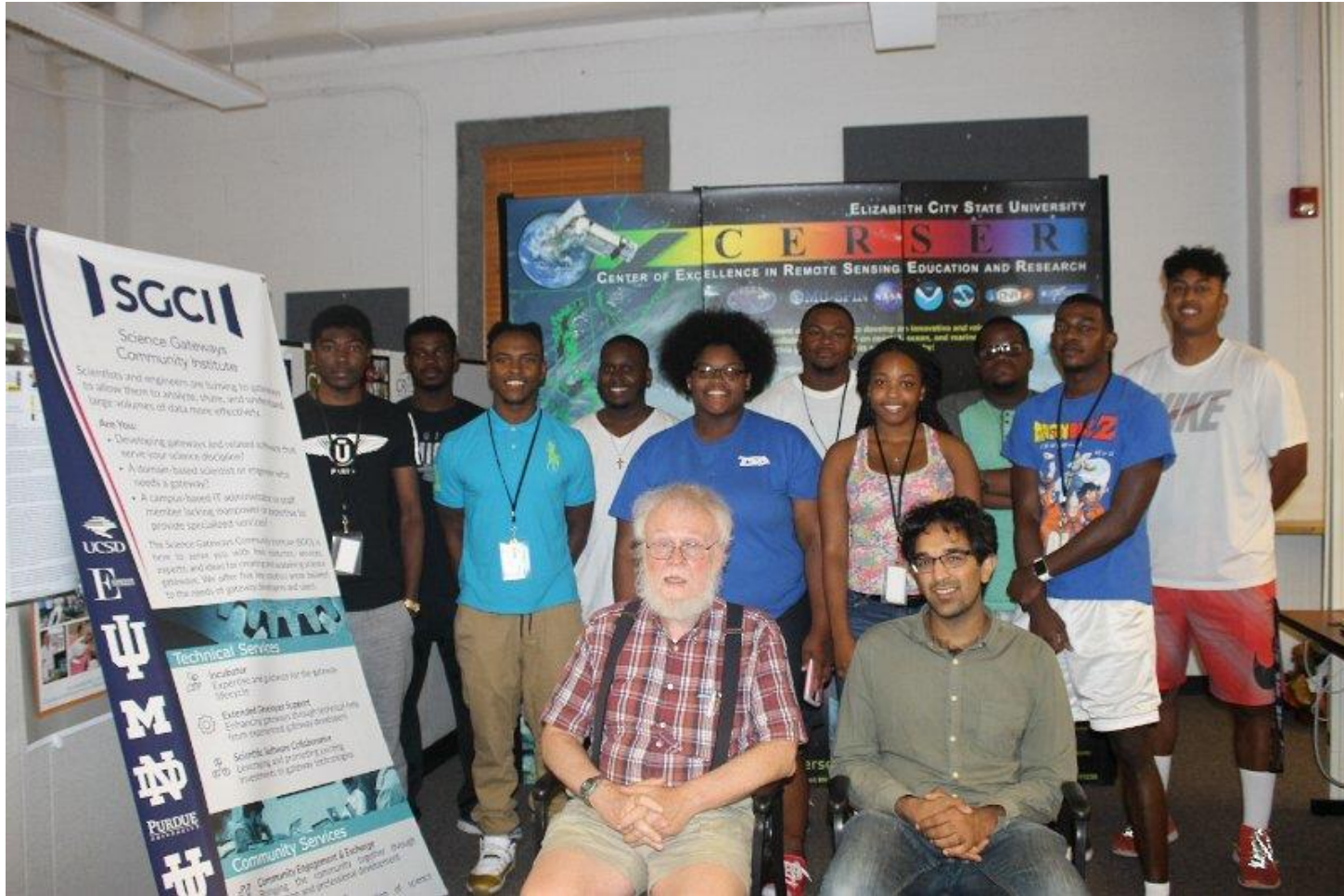


# PRESENTERS

- Linda Bailey Hayden, SGCI - ECSU
- Sudhakar V Pamidighantam, SGCI – IU
- Jerzy Leszczynski, JSU
- Teresa Head-Gordon, MoISSI
- Yassin Jeilani, Spelman College
- Vince Ortiz, Auburn University
- Robert Cave, NSF
- Suresh Marru, SGCI- IU



# 4-week Coding Institute



# 4-week Coding Institute



Mahamat Oumar and Ke'Darius Whitley of  
Winston-Salem State University  
Jeffrey Guzman, Saint Augustine's University



Students were introduced to the Software Carpentry team as well as new programming languages. During the Software Carpentry tutorials the students were introduced to git bash and GitLab.com. The students were taught how to use the Linux terminal to navigate GitLab.com and how to save their work. The students also learned other programming languages such as R, Python, and Unix Shell.



La'Andrea Gates, Kartavis Phillips,  
Kyanie Waters  
Mississippi Valley State University

# 4-week Coding Institute



Derek Morris and Reginald Kelley  
Elizabeth City State University

Edsel Norwood II  
College of the Albemarle

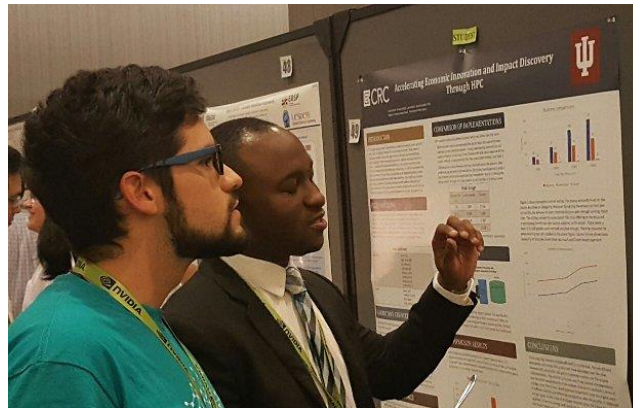


Students traveled to New Orleans to attend the PEARC17 conference, participated in a student modeling competition and Science Gateway tutorials.

# PEARC17

# Student Papers and Posters

Student papers and posters were a great opportunity to meet others both in and out of their field during the PEARC17 program and a chance to discuss their work in greater detail with conference attendees and exhibitors.



# Gaining Valuable Modeling Experience



During Modeling Day, students worked in teams to build a model of a scientific phenomenon to understand its behavior and simulate a range of conditions. Teams were challenged to understand the underlying model and the simplifications it makes concerning the real system. They wrote and tested the computer codes needed to solve the problem, added additional sophistication to the models, improved the user interface to the code, and validated the code against real data or more sophisticated models. Students prepared for Modeling Day with targeted PEARC17 tutorials on Monday, and the primary modeling activity happened all day Tuesday.