Final Presentations

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Cooper Library Digital Resources Laboratory

1:30 PM – 3:30 PM

Clemson Computing and Information Technology

Clemson University

July 25, 2014

REU Site
Collaborative Data Visualization Applications

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Congratulations to all of the 2014 VisREU Students Attending XSEDE14!

2014 VisREU Students

Michael Bosch	Poster Presentation
Colleen Burns	Poster Presentation
Cameron Collins	Poster Presentation
Kenneth Curtis	XSEDE14 Travel Scholarship Recipient
Luther Fant	Poster Presentation
Hali Gallagher	XSEDE14 Travel Scholarship Recipient
Mokell Moses	XSEDE14 Travel Scholarship Recipient
Asher Sampong	Sponsored by CCIT
Tyler Slonecki	Poster Presentation

REU Site
Collaborative Data Visualization Applications

Intelligent River Viewing Room
Mokell Moses
Research Mentor: Dr. Jason Hallstrom
Visualization Mentor: Dr. Jill Gemmill
1:30 PM – 1:35 PM

The Savannah River Basin in South Carolina has been chosen as the focus of a very special project. The Intelligent River Viewing Room targets the data that the river can provide. With a spacious room and multiple high resolution screens and projectors, the River Room provides the sense that a person is actually taking a trip down the river. Sensors are placed at separate points in the river and they transmit the data that they collect back to the room. Information then displays and the river can be observed and judged without anyone ever having to visit the wet banks. The data is interesting and diversified and the decisions about the river can be made. The location of sensors is represented on a map of the river that appears in the room; clicking on the locations displays data being collected at that location.

Expressing Sustainability within the Web-Based Multiplayer Game *Naranpur Online*
Michael Bosch
Mentors: Dr. Stephen Moysey; Dr. Catherine Mobley; Dr. Matthew Boyer
Visualization Mentor: Dr. Vetria Byrd
1:40 PM – 1:45 PM

Since the concept of sustainability is fairly abstract, it is often difficult to depict to others whether a region is undergoing sustainable development. One solution is to develop and visualize a system of metrics and indicators that measure the sustainability of a region. This can pose a challenge, as regions have differing aspects that indicate sustainable development, thus making it hard to develop universal indicators that can be applied across regions. *Naranpur Online*, an online multiplayer watershed management game, simulates an agricultural environment where players interact to impact the potential of a region to evolve as a "sustainable system." For this project, I have developed seven metrics, each containing several indicators, which will be able to determine the relative sustainable development of both the entire world of Naranpur and the individual player's farming property. These metrics are used within a "hierarchical metrics system," such that there are three tertiary metrics (economy, society, and environment), three secondary metrics (eco-economic, socio-environmental, and socio-economic), and one primary metric (eco-socio-economic), where the primary metric has priority over the other two metric types in assessing sustainable development. Being able to visualize sustainable development within Naranpur will facilitate a player's understanding of the concept of sustainability and how they themselves contribute to a more global sustainable development.

Visualization to Enhance Rare Event Simulations of Ice Nucleation
Tyler Slonecki
Research Mentor: Dr. Sapna Sarupria
Visualization Mentor: Dr. Joshua Levine
1:50 PM – 1:55 PM

Normally, small impurities within water facilitate the freezing of water. Theoretically, pure water forms ice clusters spontaneously after reaching low temperatures. However, there is not currently a way to purify water of 100% of these impurities. Thus, determining how completely pure water freezes would be difficult to explain experimentally. Through molecular dynamics simulations combined with Forward Flux Sampling (FFS) technique to overcome computationally expensive direct molecular dynamics simulations, it is possible to computationally imitate freezing of pure water. These computations produce large amounts data that make patterns difficult to interpret. Visualization of this data helps provide insight into patterns and how pure water freezes. Parallel coordinates is a useful visualization tool that allows for multidimensional comparison of different criteria calculated from the data.

Specifically, an expanded parallel coordinates tool is particularly useful for this project because it allows for comparison of different measures within the data while also providing other tools to analyze those specific comparisons. Alteration of a parallel coordinates program named EDEN has resulted in a visualization tool with many new features that allow for better analysis of how pure water freezes. Additional visualization tools that stem from the modified EDEN allow for additional analysis of particular simulated molecular formations. Ultimately, this tool will help determine optimal conditions that allow pure water to freeze with eventual hopes that it can be used to determine how environmental conditions affect phase transitions in aqueous systems.

Modernists' Letters: A Journey into the Modernist Mind

Hali Gallagher
Research Mentor: Dr. Gabriel Hankins
Visualization Mentor: Dr. Jill Gemmill
2:00 PM – 2:05 PM

This research looks at the letters from the modernist writers Scott Fitzgerald and Ernest Hemingway. The goal in this project is to make clearer connections between these two writers through the use of the visualization tool Palladio. The data was collected by reading and entering metadata into table format, and then exporting it into Palladio. The metadata includes the letter ID, author of the letter, letter recipient, date the letter was written, destination place, author place, letter type, where the original letter is archived, and the reference page from secondary source. With Palladio, it can be seen exactly where the letters were sent with a map visualization. Palladio can also display connections through the creation of a string graph. The visualization shows that each writer had connections in both America and Paris. The data also concludes these writers made connections with other influential writers of their time period. Inferences from the data reflect Fitzgerald and Hemingway's desire to further their career through networking.

Visualization of Biomedicinal Organometallic Crystal Structures and Molecules

Kenneth M. Curtis
Research Mentor: Dr. Andrew Tennyson
Visualization Mentor: Dr. Jill Gemmill
2:10 PM – 2:15 PM

This project involved creating compounds that improve effectiveness of treatment methods when previously, diseases were multidrug resistant. Complexes of silver and gold supported by N-heterocyclic carbene (NHC) ligands have recently been found to show effectiveness against different diseases resistant to normal medication but cannot be modified for bio-conjugation of cell-trapping. Gold and silver have properties that prevent cell damage when they bind with chemicals in the blood. By putting focus on cleating NHC ligands which bind metals with more than one atom, new classes of cleating NHC ligands were created. Silver and gold have the geometric requirement of being able to only bind a ligand at two sites 180 degrees apart. The visualization models illustrate details like bond angles that previously were not conveyed using conventional methods like pictures or sketches. Programs like *Chimera* and *Jmol* made it possible to create representations of these structures for further analysis. *Chimera* can be used when making videos of 3D models whereas *Jmol* excels in interacting and manipulating the 3D structures. Since molecules often have many different bond angles and can change structurally as they interact with other atoms and molecules, it is important to be able show these changes and interactions.

Light Visualization in the Dominican Rainforest

Colleen Burns
Research Mentor: Dr. Saara DeWalt
Visualization Mentor: Dr. Vetria Byrd
2:20 PM – 2:25 PM

The objective of this research is to use visualization tools to identify trends in

understory light levels in the Dominican rainforest, as well as to evaluate the effectiveness of hemispherical photos as an indirect measure of light. Three quantum light sensors measuring photosynthetically active radiation (PAR) were placed in each of nine forest plots. Each sensor measured the light level every 10 seconds, and these readings were averaged and recorded over five-minute intervals using a datalogger. A hemispherical photo was taken at each sensor location using a fisheye lens, which captured a complete view of the canopy cover above each PAR sensor. The photographs were processed using Gap Light Analyzer (GLA), which returned various indirect measurements of light levels, including Percent Canopy Openness. R (statistical package) was used to subset PAR sensor data by month and to perform basic analysis, including finding the average light level for each sensor and identifying statistical outliers. To gain additional insight, Tableau was used as a tool to visualize patterns in light levels across a time period. Readings were plotted from each PAR sensor for the month of June 2008 and filtered by forest site. This visualization allowed the researchers to recognize features of the data that had not previously been apparent.

El Purgatorio

Kayla DiMarco
Research Mentor: Melissa Vogel
Visualization Mentor: Vetria Byrd
2:30 PM – 2:35 PM

Anthropological researchers have collaborated with archaeologists to understand the pre-Columbian city, El Purgatorio. Archaeologists cannot excavate the entire urban environment and must strategically dig in select areas. Open-source 3D modeling software is being used in this project to piece together the field notes, photographs, and CAD drawings gathered from the excavation sites. The 3D software, Blender, provides a navigable view of the entire compound that Dr. Vogel can show to anyone what this ancient society looked like to its citizens. These visualizations can answer the questions that have been left without answers by recreating this ancient world in the modern day. These visualization tools help anthropologists to better understand the historical implications of the ancient architectural designs.

Visualizing Gene – Interactions within the Rice and Maize Network

Asher Sampong
Research Mentor: Dr. Alex Feltus
Visualization Mentor: Dr. Joshua Levine
2:40 PM – 2:45 PM

The purpose of this research was to design a simpler visualization tool for comparing or viewing gene interaction graphs in systems biology. This visualization tool made it possible and easier for a researcher to visualize the biological metadata of a plant and interact with the graph on a webpage. Although there are current visualization software like *Cytoscape* and *Walrus*, they are difficult to interact with and do not scale effectively when given a large data set, limiting the ability to visualize interactions within a biological system. The visualization program tool being developed will be very useful when viewing and interpreting the dataset of a gene interaction network. The graph layout drawn by this visualization tool will be an improvement from comparing lines of genes in two separate data files to, now having the ability to visually see the layout of the gene networks and how the two systems are related. For the purpose of this research, the graph layout presented by the visualization tool will draw a graph of the rice gene and maize gene network, linking the common genes found in both plants and highlighting the functions served by common genes from each plant. The success of this visualization tool will enable Dr Feltus to continue his investigations and draw conclusions on the biological evolution of the sorghum plant as well.

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Visualizing the Properties of Carbon-based Molecules

Cameron Collins

Research Mentor: Dr. Steve Stuart
Visualization Mentor: Dr. Joshua Levine
2:50 PM – 2:55 PM

Most visualization tools used in chemistry are capable of visualizing basic properties such as bond distance, angle, etc, but lack the ability to visualize other more specific properties. The software developed as a result of this project, measures both the chemical and mathematical properties that are exclusive to carbon-based molecules. *Processing* is a graphics-based programming language that uses *Java* syntax to build the software. The first step involved reading the file provided and developing a three-dimensional model. Next a *Processing* library was imported which allows the user to rotate and zoom in on the model. The final step was to develop a user interface which allows the user to select which properties that he/she wants displayed, which will color the atoms, bonds, and rings based upon those properties. All of the properties being visualized are either very difficult to see without computer simulation making the use of color necessary. Future work will involve transferring the software to a language that is more reliable, such as *Python*, and to make a more user-friendly graphical interface.

2014 VisREU Students	**Home Institution**
Michael Bosch	University of South Dakota
Colleen Burns	University of Arkansas
Cameron Collins	Coastal Carolina University
Kenneth Curtis	University of Alabama at Birmingham
Kayla DiMarco	Clemson University
Luther Fant	Clemson University
Hali Gallagher	Coastal Carolina University
Mokell Moses	Norfolk State University
Asher Sampong	Fort Valley State University
Tyler Slonecki	Wofford College

Virtualizing the Real-World for Environmental Education using the Oculus Rift

Luther Fant

Research Mentor: Dr. Stephen Moysey,
Research Mentor: Dr. Matthew Boyer
Visualization Mentor: Dr. Vetria Byrd
3:00 PM – 3:05 PM

A lack of local accessibility and availability of real-world environmental sites is a significant problem for engaging students and the public in fields such as geology. In this project we are investigating whether 3D virtual reality tools and real-world geographic data can be used to create authentic, interactive environmental education experiences. This Project undertakes the task by recreating real world environments in a virtual setting using the Unity 3D engine and Oculus Rift. The Oculus Rift has received wide attention as one of the first piece of hardware capable of producing authentic virtual reality experiences. We demonstrate the potential of this device for environmental education by rendering topographic data of the Grand Canyon provided by the United States Geological Survey. Using the Oculus Rift, a user is able to fly through the Canyon on a virtual tour designed to highlight geologic features of interest. In addition to observing the topography of the Canyon, it is also possible to augment the scene with aerial photos and supplemental data (such as layering the landscape with geologic maps). As a result, users obtain a unique experience that links the sensation of observing real geography with educational content in a way that could not be achieved in the real world. Development of environmental applications for emerging virtual reality tools is therefore likely to improve learning opportunities in environmental education, particularly for those that would otherwise not have the opportunity to experience real-world environments in person or in situations where concepts could not be communicated effectively in the field.