

# Update on Computational Efforts UCO

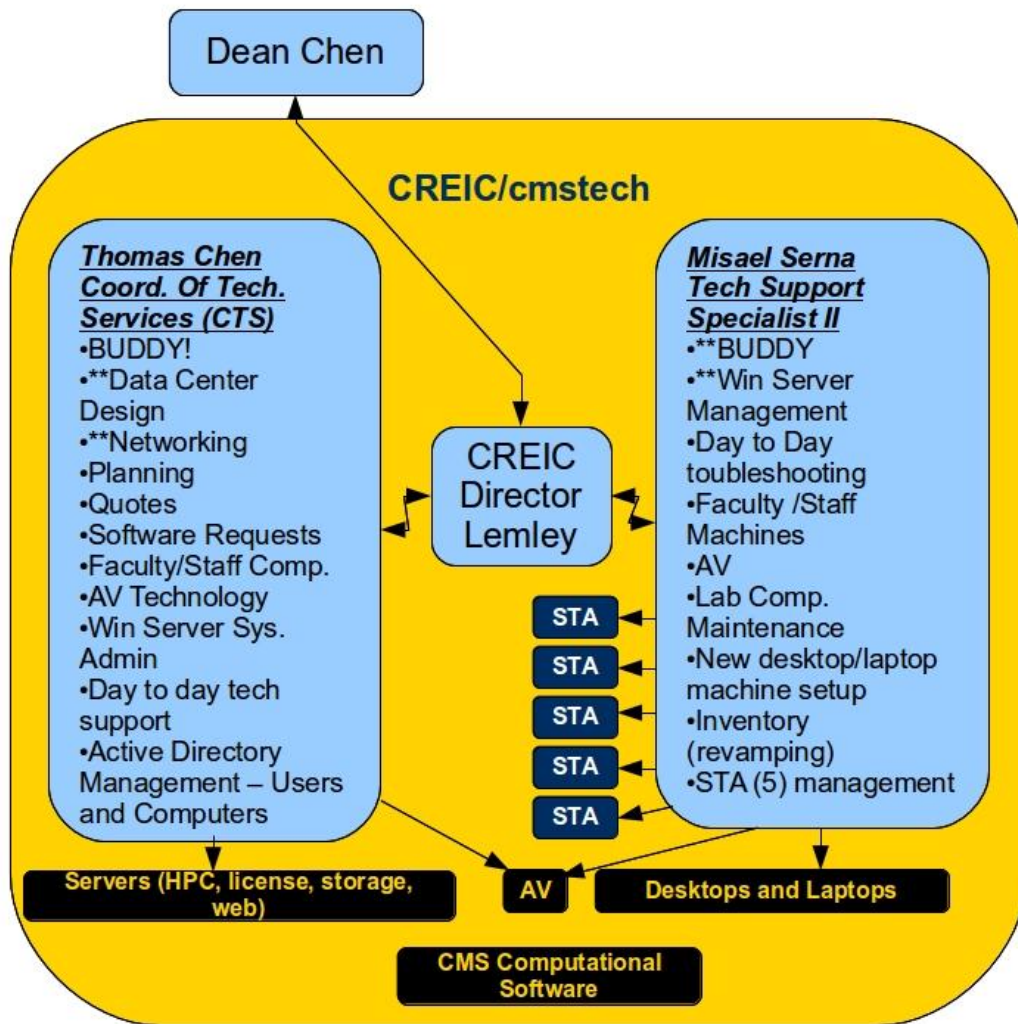
*Oklahoma Supercomputing Symposium  
Sept. 21, 2016*

Evan Lemley  
Thomas Chen  
Ivan Gutierrez



UNIVERSITY OF CENTRAL OKLAHOMA

# UCO College of Mathematics and Science



# CREIC (Center for Research and Education in Interdisciplinary Computation)

## ● UCO's first HPC Center

- 2007 3-node Cluster (Penguin Computing)
  - Xeon 65 nm dual core
- 2010 6-node desktop PCs
- 2013 Dell R520 server
- Buddy!
  - NSF MRI (ACI #1429702)
    - \$304,745
    - MRI: Acquisition of a High Performance Computing Cluster for Research at a Predominantly Undergraduate Institution
    - Vendor = Advanced Clustering Technologies
    - Deployed July 2015



# Buddy

- Hardware

- 31 General Purpose Nodes

- Dual Xeon 10-core (Haswell)
- 64 GB RAM

- 4 Hi-Mem Nodes

- Dual Xeon 10-core (Haswell)
- 128 GB RAM

- 2 GPU Nodes

- Dual Xeon 10-core (Haswell)
- 64 GB RAM
- 1 GPU Card (NVidia Tesla K40)
- 2 Xeon Phi cards



# Buddy

- Hardware

- Storage Node

- Dual Xeon 8-core (Haswell)
- 64 GB RAM
- 64 TB of Drive Space! (more like 50 TB formatted into RAID6)

- Network

- Gb Ethernet - 1 Gb/s *Management*
- Infiniband -- 40 Gb/s *Messages*
  - 1000x-4000x US High Speed Downloads
  - This is how the cluster acts like a single computer



# ● NSF MRI

## ○ Buddy Projects

Perceptual Optimization of X-ray Fluoroscopy (Biomedical Imaging)

Fluid Flow in Microchannel Junctions - Entropy Generation for Fluid Energy Losses (Microfluidics)

Parallelization of the NSP-Tree (Bioinformatics)

Janus Particle Transport in Microfluidics & Selective Electromagnetic Heating (Microfluidics & Bioheat Transfer)

An Intelligent System for the Disabled (Intelligent Systems / Neural Networks)

Design of Intervertebral Discs (Biomechanics)

Biomechanics of Cilia and Flagella (Biomechanics)

Ecological Niche Modeling (Computational Biology)

Population Genetics (Phylogenetics)

Liquid Crystal Modeling (Elect. Engr.)

Recognition of Conserved Protein Sets Among Photosynthetic Eukayotes to Determine Evolutionary and Biochemical Relationships (Bioinformatics)

Permutation Test for a Covariance Matrix (Statistics)

Geometry optimization of aerodynamic add-on devices on road vehicles (aerodynamics)

Spread of Disease in Structured Host Populations (Mathematical Biology)

Modeling of Energy Absorption and Heat Transport in Laser Tumor Irradiation (Bioheat Transfer)

Operations Research Clinic (Mathematics)

Modelling fibrinolysis: a 3D stochastic multiscale model (Mathematical Biology)

Class Implementation + Other UCO Research + Outreach + OneOCII



# Buddy



# Buddy

- Software

- Management

- ACT\_Utils
- SLURM
- Ganglia

- Applications (some of them)

- ANSYS (*New licensing*)
- COMSOL (*New licensing*)
- Matlab (*New licensing*)
- Mathematica
- Compilers - for homegrown software
- R
- ...





# Buddy



- Initial Deployment - June/July 2015
- Software Installs & Testing - Aug/ 2015 - current
- Users:
  - Sept. 2015 -- 7
  - Sept. 2016 -- > 70
    - Faculty + Students
- Research:
  - ~5 Papers:
    - Hossan, Fenwick, Lemley, ...
- Grants:
  - 4 grants:
    - Genetics, Microfluidics, Forensics, Species Hybridization
- Classes:
  - Used in >4 classes.
    - PDE's, Biological Math, Computational Science, Engineering Stats.



# Buddy



- New Connection Directly to OneNet
  - 10 Gbps dedicated network
  - Access from anywhere
  - Web interface
- Future Connection to OFFN
  - Oklahoma Friction Free Network
- Planned use for ATLAS
  - High energy physics research working with LHC Data
- Training
  - Weekly and deskside help sessions in Spring 2016
  - Continue in Fall 2016

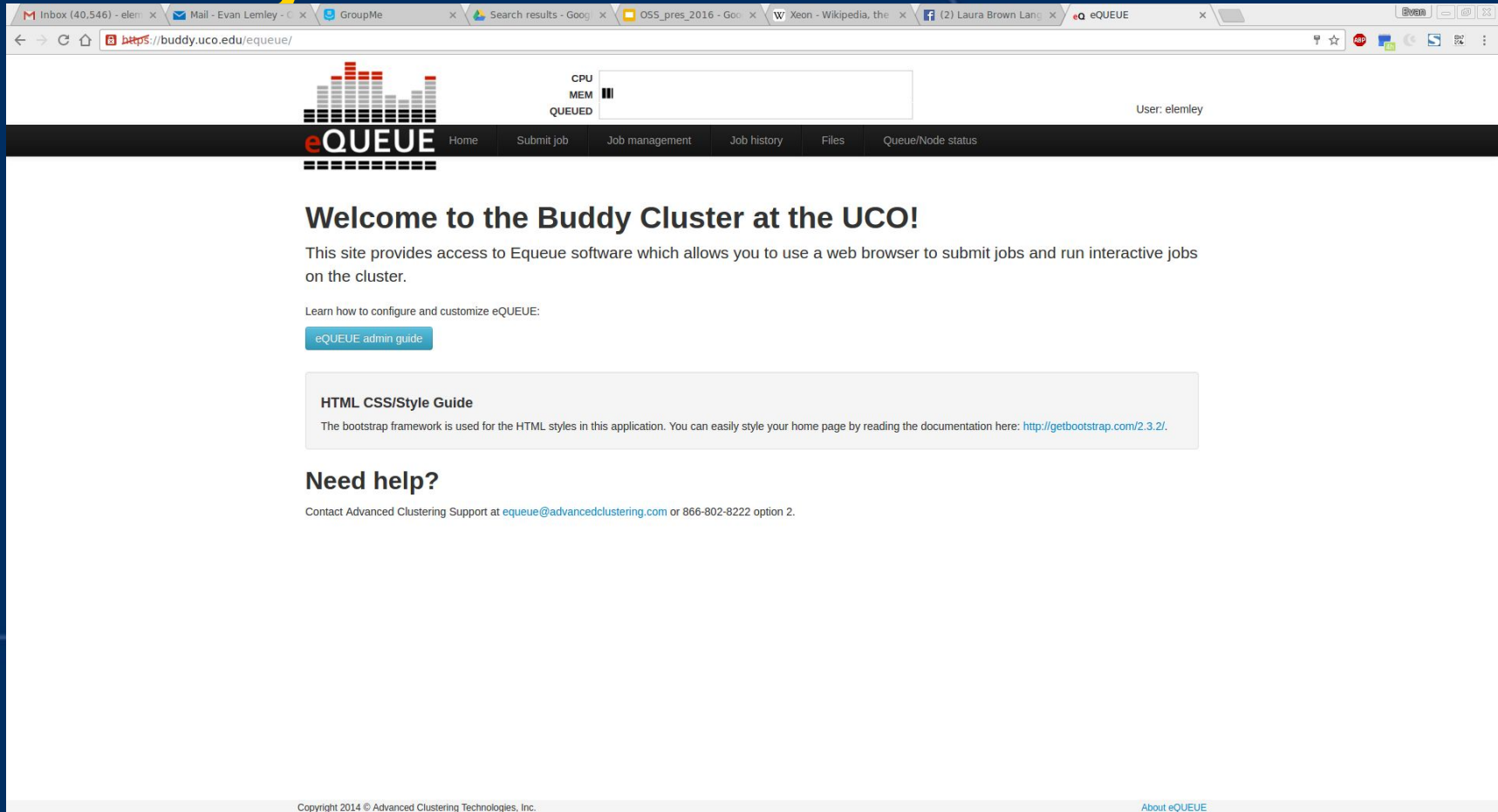


# Buddy

- Access
  - ssh
    - PKI
      - Automated setup for Windows, Mac, Linux
      - Key generated locally and uploaded
  - Browser-based
    - eQUEUE (Advanced Clustering Technologies)
    - TurboVNC-based sessions



# Buddy



The screenshot shows a web browser window with the URL <https://buddy.uco.edu/equeue/>. The page features a header with the eQUEUE logo, a navigation menu (Home, Submit job, Job management, Job history, Files, Queue/Node status), and a user profile (User: elemley). The main content area includes a welcome message, a link to the eQUEUE admin guide, and a section for the HTML CSS/Style Guide. The footer contains copyright information and a link to the About eQUEUE page.

**eQUEUE** Home Submit job Job management Job history Files Queue/Node status

User: elemley

## Welcome to the Buddy Cluster at the UCO!

This site provides access to Equeue software which allows you to use a web browser to submit jobs and run interactive jobs on the cluster.

Learn how to configure and customize eQUEUE:

[eQUEUE admin guide](#)

### HTML CSS/Style Guide

The bootstrap framework is used for the HTML styles in this application. You can easily style your home page by reading the documentation here: <http://getbootstrap.com/2.3.2/>.

## Need help?

Contact Advanced Clustering Support at [equeue@advancedclustering.com](mailto:equeue@advancedclustering.com) or 866-802-8222 option 2.

Copyright 2014 © Advanced Clustering Technologies, Inc. [About eQUEUE](#)



# Buddy

The screenshot shows a web browser window with the URL <https://buddy.uco.edu/equeue/>. The page features a navigation bar with the eQUEUE logo and links for Home, Submit job, Job management, Job history, Files, and Queue/Node status. A user profile for 'User: elemley' is visible in the top right. The main content area is titled 'Submit a Job' and includes a breadcrumb path: 'Path: Forms / Desktop\_Apps'. A list of application categories is provided, each with a description:

- BEASTv1.8.2**: Submit a BEASTv1.8.2 GUI Job
- BEASTv2.3.2**: Submit a BEASTv2.3.2 GUI Job
- Comsol**: Start a COMSOL session
- Desktop**: Start a full GNOME desktop session
- Firefox**: Start a firefox session
- Fluent**: Start a Fluent session
- GEdit**: Edit text files
- GalaxSee**: Use GalaxSee on the cluster
- Galaxy**: Start a Galaxy session
- Mathematica**: Start a Mathematica session
- Matlab**: Start a MATLAB 2016A session
- Netanim**: Start a NetAnim Session
- Python**: Start a Python IDLE session
- Rstudio**: Start a Rstudio session
- StacksWeb**: Start a Stacks Web GUI session
- Structure**: Start a Structure session
- Visit**: Start a Visit session
- Weka**: Submit a Weka Job
- Workbench**: Start an ANSYS Workbench session

At the bottom of the page, there is a copyright notice: 'Copyright 2014 © Advanced Clustering Technologies, Inc.' and a link for 'About eQUEUE'.



# CREIC (Center for Research and Education in Interdisciplinary Computation)



## Plans

- New Academic Data Center in Interdisc. STEM Bldg.
  - Currently working with OIT, Engr. Firm, and vendor on design.
  - Equipment/Infrastructure
    - UPS
    - Generator (bldg.)
    - Cooling
    - Rack Arrangement
    - Planning for Growth
- Computational Classroom
  - Design Phase



# PSM Program

- Approved by Regent's in June 2016
- Website: [psm.uco.edu](http://psm.uco.edu)
- Very basic marketing for Fall
- Small student cohort in Fall
- Start a new cohort in Spring 2017
- PSM Computational Science
  - Computer Science
  - Computational Engineering
  - Computational Mathematics

*Not an M.S. it's officially a P.S.M.*



# PSM Program

- STEM+Business
- Developed with Industry Input
- No Thesis Required (a real world project is)
- Flexibility and Convenience
- Low Cost / High Quality





# PSM Program

- PSM classes running this Fall
  - Computational Science for Prof. I
    - Will Holmes - UCOdowntown
  - Will Holmes - 17 years of engineering and physics faculty experience



# PSM Program Plans

- Develop PSM classes as blended classes for Year 2
- Strong Industry Partners
- Gather feedback from OKC Employers
- Develop Projects with OKC Employers
- Assistantships (2) per the Proposal
  - ~\$15k/year
- Software for CSP and Capstone Projects
  - ~\$2k/year



## Discussion

- Questions?
- Feedback?

Evan Lemley

[elemley@uco.edu](mailto:elemley@uco.edu)

405-974-5473



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