

NSF Award No. OIA-1301789 "Adapting Socio-Ecological Systems to Increased Climate Variability"



Oklahoma NSF EPSCoR State Conference

April, 2017



OKLAHOMA NSF EPSCoR STATE CONFERENCE

The OneOklahoma Cyberinfrastructure Initiative

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Outline

- OneOklahoma Cyberinfrastructure Initiative (OneOCII)
- Informatics & TIGER: The Interactive Graphical Environment for Research

Materials developed by the EPSCoR Project's Cyberinfrastructure Team:

- Henry Neeman & Mark Stacy, University of Oklahoma
- Dana Brunson & Evan Linde, Oklahoma State University



OneOK Cyberinfrastructure Initiative

- Created via MOU in OK's NSF EPSCoR RII Track-1 2008-13, then expanded under OK's RII Track-1 2013-18.
- All academic institutions in Oklahoma are eligible to sign up for free use of OU's and OSU's centrally-owned Cyberinfrastructure resources.
- Other kinds of institutions (government, non-governmental) are eligible to use, though not necessarily for free.
- Everyone can participate in our CI education initiative.
- The Oklahoma Supercomputing Symposium, our annual conference, continues to be offered to all.





AAAS report, April 2016

"From a scientific collaboration/integration perspective, three accomplishments are noted by the Panel. The first is the **OneOCII between** OU and OSU, and a true 'jewel in the EPSCoR crown.' It serves as a model for what a highly successful and supportive collaborative effort could produce. It is particularly noteworthy in that it enables the free usage of all OU and OSU centrally owned CI by all Oklahomans. One best practice that has proven valuable has been the early embedding of CI in all elements of the conducted research, enabling the research goals to be met. Another is the training sessions and support (e.g. software carpentry and workshops on the use of downscaled climate data) by all users, not only EPSCoR-funded researchers. Open access is also facilitated by the use of virtual machines and cloud operations for pivotal frameworks such as ENVISION, providing strong support of collaborative research efforts. This collaboration and its best practices have attracted national NSF interest in terms of disseminating this success at the national scale."



OneOCII Goals

- <u>**Reach</u>** institutions outside the mainstream of advanced computing.</u>
- <u>Serve</u> every higher education institution in Oklahoma that has relevant curricula.
- **Educate** Oklahomans about advanced computing.
- <u>Attract</u> underrepresented populations and institution types into advanced computing.



• <u>Access</u>: to supercomputers and related technologies (20 OK academic institutions to date).

Dissemination:

- Oklahoma Supercomputing Symposium annual advanced computing conference has reached 112 academic institutions, 143 commercial, 36 government, 20 nongovernmental (25 OK academic institutions to date).
- CADRE Spring Conference Coalition for Advancing Digital Research & Education brings together CI experts, Librarians, researchers and educators. Inaugural Conference April 11-12, 2017 with over 170 preregistered from 20 academic institutions, 11 commercial, 8 government, and 3 nongovernmental (14 OK academic institutions.)



<u>Education</u>: "Supercomputing in Plain English" (SiPE) workshop series: 11 talks about advanced computing, taught with stories, analogies and play rather than deep technical jargon. Have reached 362 institutions (academic, government, industry, nonprofit) in 51 US states and territories and 17 other countries (16 OK academic institutions to date).



- <u>Faculty/Staff Development</u>: Workshops held at OU and OSU on advanced computing and computational science topics, sponsored by the National Computational Science Institute, the SC supercomputing conference series, the Linux Clusters Institute, the Virtual School for Computational Science & Engineering. Oklahoma is the only state to have hosted multiple events sponsored by each of these (18 OK academic to date).
- **Informatics**: research facilitators embedded in specific research projects (and largely funded by them).
- <u>Outreach</u>: "Supercomputing in Plain English" (SiPE) overview talk (25 OK academic to date).



- <u>Proposal Support</u>: Letters of commitment for access to OneOCII resources; collaborations with OneOCII lead institutions (8 OK academic, 1 nongovernmental).
 - Helped Northeastern State U, Southeastern Oklahoma State U, Southwestern Oklahoma State U and Rogers State U submit their first NSF proposal for research networking.
- <u>Stewardship</u>: Research data stewardship initiative, led by OSU and OU Libraries.
- <u>**Technology</u>**: Got or helped get technology (e.g., network upgrade, mini-supercomputer, hi def video camera for telepresence) for that institution (14 OK academic to date).</u>
 - OSU donated some of their older supercomputer's servers to Southeastern Oklahoma State U, Southwestern Oklahoma State U.



- **Workforce Development** (39 OK academic)
 - Oklahoma Information Technology Mentorship Program (OITMP)
 - "A Day in the Life of an IT Professional" presentations to courses across the full spectrum of higher education.
 - Job shadowing opportunities and direct mentoring of individual students.
 - Institution Types: high schools, career techs, community colleges, regional universities, PhD-granting universities.
 - Special effort to reach underrepresented populations: underrepresented minorities, non-PhD-granting, especially rural institutions.



- NEW: Software & Data Carpentry: OSU & OU offer multiple Software/Data Carpentry workshops each year and train new instructors, available to all Oklahomans.
- **NEW: Research Facilitators**: 1.5 FTE hired at OU to work with researchers (but funded internally and not embedded).



OneOCII Institution Profile

To date, OneOCII has served 103 Oklahoma institutions, agencies and organizations:

- 55 OK academic
 - Universities & Colleges
 - 3 comprehensive PhD-granting
 - 20 regional non-PhD-granting
 - Community Colleges: 10
 - Career techs: 14
 - Secondary schools: 4
 - Public school systems: 4
 - Preschool: 1
 - Homeschool group: 1



OneOCII Institution Profile

Minority Serving Institutions

- Oklahoma's <u>Historically Black College or University</u>
 - Langston University (Langston)
- <u>Native American Serving Non-tribal Institutions</u>
 - East Central University (Ada)
 - Northeastern Oklahoma A&M College (Miami)
 - Northeastern State University (Tahlequah)
 - Southeastern Oklahoma State University (Durant)
- Tribal Institutions
 - College of the Muscogee Nation (Okmulgee)
 - Comanche Nation College (Lawton)
 - Pawnee Nation College (Pawnee)
 - Sequoyah High School
- Other Minority Serving Institution
 - Bacone College (Muskogee)
- Plus 16 others with above average for one or more underrepresented minorities



OneOCII Institution Profile

- 48 OK non-academic (including commercial, government, military, NGOs)
 - 16 commercial
 - 19 government
 - 2 military
 - 11 non-governmental



OneOklahoma Cyberinfrastructure Initiative



OneOCII Outcomes: Research

- External research funding to OK institutions facilitated by OneOCII lead institutions (Fall 2001- Spring 2016): \$200M+
- Funded projects facilitated: **300**+
- OK faculty and staff: **200**+ in **20**+ academic disciplines
- Specifically needed OneOCII just to be funded: ~\$44M
- NSF Major Research Instrumentation for CI: OU, OSU, Langston Univ., Univ. of Central OK, TU
- NSF Networking Grant Collaborations: OU, OSU, TU, Langston Univ., SRNF, Onenet, Univ. of Central OK
- Publications facilitated: over 2000



OneOCII Outcomes: Education

Teaching: 9 institutions including 3 MSIs

- Taught parallel computing using OneOCII resources:
 - <u>Cameron University</u> multiple times
 - <u>East Central University</u> (NASNI)
 - <u>Oklahoma City University</u> multiple times
- Taught parallel computing via LittleFe baby supercomputer and OneOCII resources:
 - <u>Southeastern Oklahoma State Univ.</u> (NASNI) 3 semester sequence, multiple times
- Taught computational chemistry using OneOCII resources:
 - Northeastern State University (NASNI) multiple times
 - <u>Southern Nazarene University</u>
 - <u>Rogers State University</u> multiple times
- Taught Bioinformatics using OneOCII resources:
 - <u>TU</u>-2 semester sequence

Several classes at OU and OSU where there are also student supercomputing clubs.



OneOCII Outcomes: Resources

- 7 institutions including 2 MSIs, plus C2 institutions
- NSF Major Research Instrumentation grants: \$2.9M
 - <u>OU</u>: Oklahoma PetaStore, \$793K (in production)
 - <u>OSU</u>: Cowboy cluster, \$909K (in production), Pistol Pete cluster, \$950K (new award)*
 - <u>Langston University</u>: cluster, \$250K (in production)
 - <u>University of Central Oklahoma</u>: cluster, \$304K (in production)*
 - <u>TU</u>: cluster, \$180K
- DOD Defense University Research Instrumentation Program
 - <u>TU</u>: cluster, \$200K
- LittleFe baby supercomputer grants (\$2520 each)
 - <u>OU</u>: Ron Barnes
 - <u>Oklahoma City University</u>: Larry Sells & John Goulden
 - <u>Southeastern Oklahoma State University</u>: Mike Morris & Karl Frinkle
- Networking
 - NSF EPSCoR RII C2 grant: \$1.17M
 - New funding
 - NSF CC-NIE grant: \$500K*
 - NSF CC*IIE grant: \$400K*



OCII/OneOCII CI Grants

Completed during this project

- NSF Grant No. ACI-10310029, "MRI: Acquisition of Extensible Petascale Storage for Data Intensive Research," OU, \$793K
- NSF Grant No. ACI-1126330, "MRI: Acquisition of a High Performance Compute Cluster for Multidisciplinary Research," OSU, \$908K
- NSF Grant No. ACI- 1229107, "MRI: Acquisition of a High Performance Computing Cluster for Research and Education," LU, \$250K

New during this project

- NSF Grant No. ACI-1341028, "OneOklahoma Friction Free Network," OU+OSU+LU+OII+UCO+OneNet, \$500K
- NSF Grant No. ACI-1440783, "A Model for Advanced Cyberinfrastructure Research and Education Facilitators," OU, \$400K
- NSF Grant No. ACI-1440774, "ENCITE: ENabling CyberInfrastructure via Training and Engagement," OneNet+GPN, \$130K
- NSF Grant No. ACI-1429702, "MRI: Acquisition of a High Performance Computing Cluster for Research at a Predominantly NSF Undergraduate Institution," UCO, \$304K
- NSF Grant No. ACI-1531128, "MRI: Acquisition of Shared High Performance Compute Cluster for Multidisciplinary Computational and Data-Intensive Research," OSU, \$950K
- DOD Grant, "DURIP-ARO: Heterogeneous Cluster for Cyber-Physical System Security Analytics," TU, \$200K
- NSF Grant No. CNS-1531270, "MRI: Development of Heterogeneous Cluster for Cyber-Physical System Hybrid Analytics," TU, \$180K

TOTAL under OCII/OneOCII: Sept. 2008-March 2016:

\$8.8M in 12 CI grants to 8 OK institutions (OU, OSU, TU, LU, UCO, OII, SRNF, OneNet)

(Average of \$1.25M per year in new CI grants to OK institutions) Comparison: 2001-2008: \$722K (3 grants), TOTAL (1/12 as much)

Papers About Pieces of OneOCII

- S. P. Calhoun, D. Akin, B. Zimmerman and H. Neeman, 2016: "Large Scale Research Data Archiving: Training for an Inconvenient Technology." *Journal of Computational Science*, to appear. DOI: <u>10.1016/j.jocs.2016.07.005</u>.
- H. Neeman, A. Bergstrom, D. Brunson, C. Ganote, Z. Gray, B. Guilfoos, R. Kalescky, E. Lemley, B. G. Moore, S. K. Ramadugu, A. Romanella, J. Rush, A. H. Sherman, B. Stengel and D. Voss, 2016: "The Advanced Cyberinfrastructure Research and Education Facilitators Virtual Residency: Toward a National Cyberinfrastructure Workforce." *Proc. XSEDE'16*, article 57.
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 K. Frinkle, Z. Gray, E. Lemley, G. Louthan, G. Monaco, M. Morris, J. Snow and B. Zimmerman, 2015:
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- S. P. Calhoun, D. Akin, J. Alexander, B. Zimmerman, F. Keller, B. George and H. Neeman, 2014: "The Oklahoma PetaStore: A Business Model for Big Data on a Small Budget." *Proc. XSEDE'14*, article 48. DOI: <u>10.1145/2616498.2616548</u>.
- C. Carley, B. McKinney, L. Sells, C. Zhao and H. Neeman, 2013: "Using a Shared, Remote Cluster for Teaching HPC." *Proc. IEEE CLUSTER 2013*. DOI: <u>10.1109/CLUSTER.2013.6702630</u>.
- H. Neeman, D. Brunson, J. Deaton, Z. Gray, E. Huebsch, D. Gentis and D. Horton, 2013: "The Oklahoma Cyberinfrastructure Initiative." *Proc. XSEDE'13*, article 70. DOI: <u>10.1145/2484762.2484793</u>.



CI Capacity

- 2002: 1.2 TFLOPs statewide, 1 Service Provider
- 2005: 6.5 TFLOPs statewide, 1 Service Provider
- 2008: 40 TFLOPs statewide, 2 Service Providers
- 2012: 200+ TFLOPs statewide, 4 Service Providers
- 2015: 400+ TFLOPs statewide, 5 Service Providers
- 2016: 500+ TFLOPs statewide, 6 Service Providers
- Plus new deployment for OSU in 2017.



National Leadership

- Workforce Development
 - OU CI lead Henry Neeman's NSF CC*IIE Campus CI Engineer grant is doing a "Virtual Residency" to teach people how to help researchers use advanced computing in their research.
 - Summer 2015 weeklong workshop: 50 CI professionals (9 from OK) participating from 38 institutions in 26 states and territories (28 onsite and 22 offsite)
 - Summer 2016 weeklong workshop: 98 participants (7 from OK) from 67 institutions in 33 states and territories plus 3 other countries (43 onsite and 56 offsite)
- NSF MRI grants
 - OSU CI lead Dana Brunson's most recent MRI has been highlighted at multiple national meetings by the Director of the NSF Advanced Cyberinfrastructure Division as exactly what the NSF wants to see from MRIs for CI.



National Leadership

- XSEDE (NSF-funded national supercomputing center program)
 - <u>Campus Engagement</u>: OU CI lead Henry Neeman and OSU CI lead Dana Brunson have been appointed XSEDE Campus Engagement Co-managers starting July 1 2016.



- Campus Champions (over 230 institutions participate so far)
- Intra-state collaboration (advise other states on benefits and help them start their own initiatives)
- Part of \$110M NSF funded XSEDE project with 19



Informatics

TIGER: The Interactive Graphical Environment for Research

TIGER - Overview

- Cloud at OSU built with EPSCoR Track I funds in 2015
- Mentorship from OU
- Powerful Windows and Linux environments for interactive use (virtual high-end workstations)
- Multi TB shared storage
- Fills the gap between desktop and HPC
- Customized configurations to meet research needs
- Over 90 registered users from OSU, OU and TU
- Many other users of resources that don't require registration

We manage the technology, you focus on your research.



TIGER - Environment

- Familiar Windows or Linux desktop (or terminal)
- Commercial software for OSU researchers and educators: ArcGIS, Matlab, SAS, ANSYS
- Open source and unrestricted software for everyone: ENVISION, LANDIS-II, R, RStudio, python, ParaView, git, QGIS, QIIME, etc.
- Adjustable resources to meet computing needs
- Training sessions as needed



TIGER - web

- JupyterHub: <u>https://jupyter.hpc.okstate.edu/</u>
 - Jupyter/IPython notebooks (Python 2/3, R, Matlab)
- GitBucket: <u>https://tiger.hpc.okstate.edu/gitbucket/</u>
 - Host private git repositories
- Shiny: <u>http://tiger.hpc.okstate.edu/sites/shiny/</u>
 - Host R Shiny apps
- Cybercommons: <u>http://data.cybercommons.org/</u>
 - Data Catalog/Repository
- Data backend for http://soilmoisture.okstate.edu/
- Many more projects serving statewide community



TIGER – Example Virtual Machines

Project Researchers

- Fieldcaster (app development Tyson Ochsner)
- Soilmapnik (web app Tyson Ochsner)
- hpc-loggernet (download data from data loggers Duncan Wilson & John Polo)

Others

- Genexpdb (web page, gene expression database Tyrrell Conway)
- hpc-ansys1(Ansys software Josh Ramsey)
- Landmark (Landmark software for geosciences Priyank Jaiswal)
- hpc-mqbiochem1 (environment with MaxQuant for proteomics group Steve Hartson)
- hpc-cloud-cars1 (GIS tools for CARS group Amy Frasier)



Ongoing Projects

- Software Carpentry multiple workshops & instructor training
- Global Climate Model Data Portal
- FUDGE Framework for Unified Downscaling of GCMs Empirically
- EcoPAD and many other Cybercommons portals
- Support for urban simulation
- Assistance with code development & data processing
- New projects on request



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 - Grant No. EPS-1006919, "Oklahoma Optical Initiative"
 - Grant No. OCI-10310029, "MRI: Acquisition of Extensible Petascale Storage for Data Intensive Research"
 - Grant No. OCI-1126330, "Acquisition of a High Performance Compute Cluster for Multidisciplinary Research"
 - Grant No. ACI- 1229107, "Acquisition of a High Performance Computing Cluster for Research and Education"
 - Grant No. EPS-1301789, "Adapting Socio-ecological Systems to Increased Climate Variability"
 - Grant No. ACI-1341028, "OneOklahoma Friction Free Network"
 - Grant No. ACI-1440783, "A Model for Advanced Cyberinfrastructure Research and Education Facilitators"
 - Grant No. ACI-1440774, "ENabling CyberInfrastructure via Training and Engagement"
 - Grant No. ACI-1531128, "MRI: Acquisition of Shared High Performance Compute Cluster for Multidisciplinary Computational and Data-Intensive Research," OSU, \$950K
 - Grant No. ?, "DURIP-ARO: Heterogeneous Cluster for Cyber-Physical System Security Analytics," TU, \$200K
 - Grant No. CNS-1531270, "MRI: Development of Heterogeneous Cluster for Cyber-Physical System Hybrid Analytics," TU, \$180K
- Dell provided seed systems for the OU Research Cloud ("OURcloud") and the OU Science DMZ.



OneOCII April 26, 2016

Thanks for your attention! Questions?

- Vendor Expo
- Poster Session April 11
- Breakout Talks April 12



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Executive Director for Science & Technology, National Center for Supercomputing Applications



Plenary Speaker Kelly Gaither, PhD Co-PI & Director of Community Engagement & Enrichment, XSEDE

Director of Visualization Texas Advanced Computing Center



