



Open Science Forum, April 26, 2017

IVMOOC on Jetstream & Open XD Metrics on Demand Value Analytics

CNS, IUNI, UITS

INDIANA UNIVERSITY BLOOMINGTON



OPEN SCIENCE FORUM

Open Science Forum

- Wednesday, Apr 26th 2017 at 4:00 PM
- SSRC Grand Hall (Woodburn Hall 200)

Jetstream, funded by NSF and led by the Indiana University Pervasive Technology Institute (PTI), adds cloud-based computation to the national cyberinfrastructure (https://jetstream-cloud.org). IUNI collaborated with the Cyberinfrastructure for Network Science Center to deploy the Network Workbench tool on Jetstream for use by IVMOOC students (http://ivmooc.cns.iu.edu).

The "Open XD Metrics on Demand Value Analytics" NSF project, directed by Matthew Link (UITS), aims to measure and visualize the impact of campus-financed cyberinfrastructure (CI) on progress in science. Resulting visual analytics modules will be added to the existing CI metrics tool eXtreme Data Metrics on Demand (XDMoD) to present a view of financial, collaboration, and publication data, showing "return-on-investment" metrics in relation to CI usage.

New Ventures in Research, Engineering, and Educational Computing.

George Turner, Chief Systems Architect Research Technologies, UITS, Indiana University

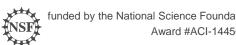
Open Science Forum, SSRC Grand Hall Indiana University Bloomington, IN 26 April 2017



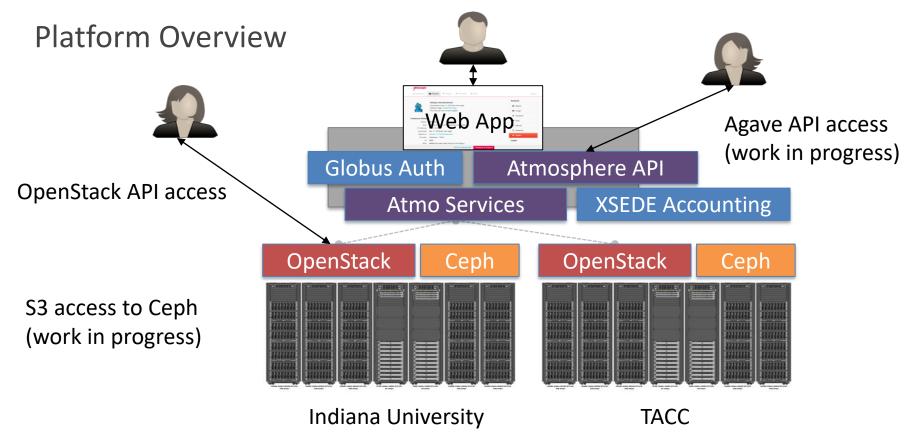
What is Jetstream?

- User-friendly, widely accessible cloud environment
 - **User-selectable library** of preconfigured virtual machines; no need for system administration skills.
 - Programmatic API access to implement modern cloud computing techniques













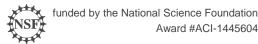




What is Jetstream?

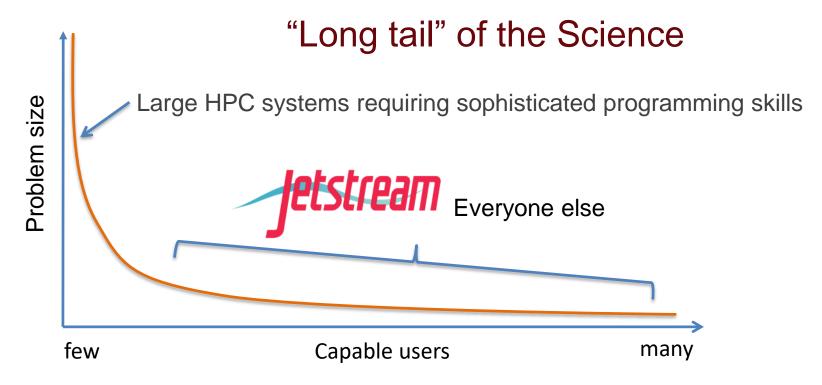
- Reproducibility: store, publish via IU Scholarworks (DOI)
- Cloudy: clouds are more the just virtual machines (VM)
 - Old way: robust (expensive) infrastructure, weak (cheap) software
 - Cloudy way: commodity infrastructure, robust software
 - Cows, not pets: pets take great amount of care, feeding, and you name them; cows you intend to have high turnover and you give them numbers.
- **Primary goal** is to **expand the user base** of NSF's eXtreme Digital (XD) program resources beyond the current community of users.







What is Jetstream? (cont)









What is Jetstream? (cont)

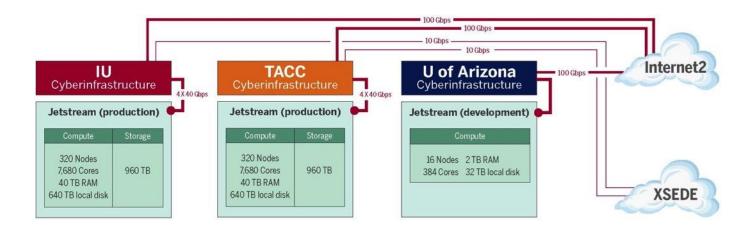
- Software layers
 - Atmosphere web interface
 - library of images, genertic, domain specific
 - simplify VM administration
 - **Openstack:** software tools for building and managing cloud computing platforms for public and private clouds.
 - KVM hypervisor: what the VMs run on
 - **Ceph**: storage platform that stores data on a single distributed computer cluster, and provides interfaces for **object**-, **block** and *file-level* storage.
 - Operating systems: CentOS, Ubuntu, Windows?
 - Applications; e.g. software developed by the domain specialist, gateways, etc.



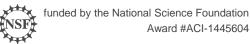




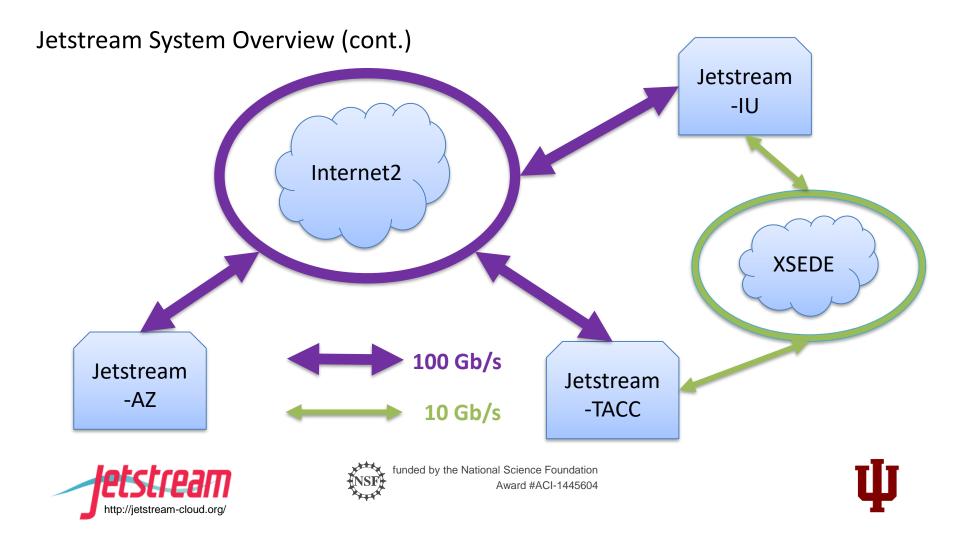
Jetstream System Overview











Production Cloud Hardware (per site)

Hardware	Number	Specifications	Function (IU)
Dell PowerEdge M630 blades	320	2X Intel E5-2680v3 "Haswell" 24 cores @ 2.5 GHz 128 GB RAM 2 TB local disk	Compute hosts OpenStack services
Dell PowerEdge R630 1U server	7	2X Intel E5-2680v3 "Haswell" 24 cores @ 2.5 GHz 128 GB RAM 2 TB local disk	Cluster management High Availability Databases RabbitMQ
Dell PowerEdge R730xd 2U servers	20	2X Intel E5-2680v3 "Haswell" 24 cores @ 2.5 GHz 64 GB RAM 48 TB storage for Ceph pool	~1 PB Ceph storage
Dell S6000-ON network switches	9	32+2 40 Gb/s ports	Top of Rack Spine







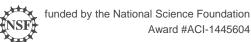
VM Instance Sizes (Flavors)

Instance Type	vCPUs	RAM(GB)	Storage(GB)	Instances/Node
Tiny	1	2	8	46
Small	2	4	20	23
Medium	6	16	60	7
Large	10	30	120/ <mark>60*</mark>	4
X-Large	22	60	240/ <mark>60*</mark>	2
XX-Large	44	120	480/ <mark>60*</mark>	1

Node config: dual Intel E-2680v3 "Haswell", 24 physical cores/node @ 2.5 GHz, 128 GB RAM, dual 1 TB local disks.

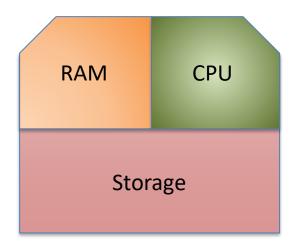
^{*} Effective 29-Mar-2017







What is an Instance

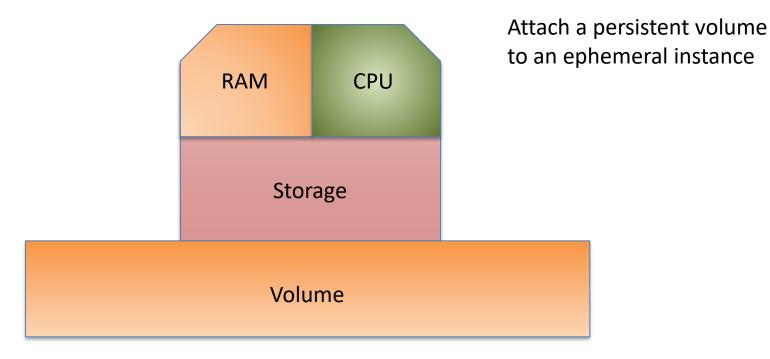




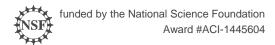




Instance & Volumes

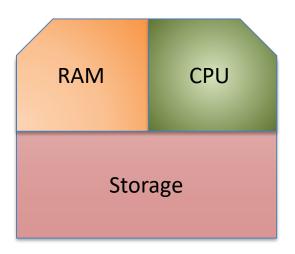








Instance & Volumes



Dettach the persistent volume to an ephemeral instance

Volume





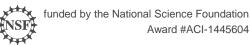


Instance & Volumes

The instance is gone but the volume persists

Volume



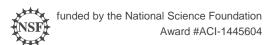




Terms

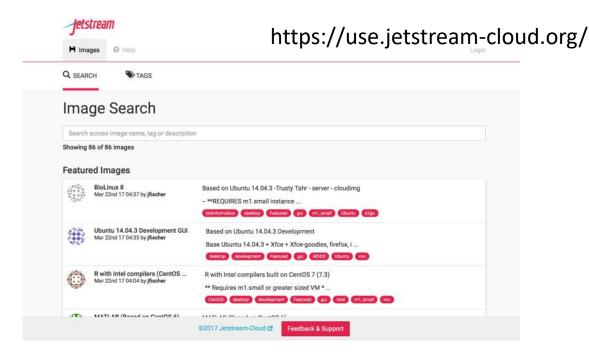
- Image: a file on a storage device
- Instance: a running
- Volumes: persistent storage device
- Flavors: the size of instance, #cpu, amt of RAM, amt of storage
- Host: hardware
- Guest:







(no login required at this point)

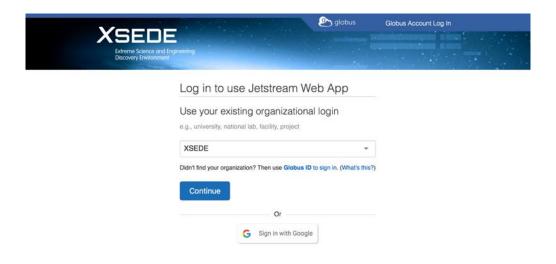




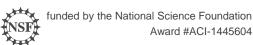




(Pick identity provider)

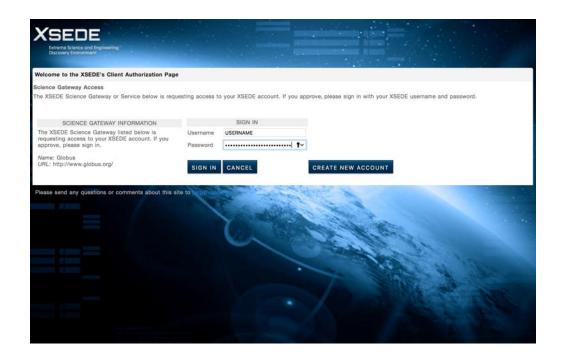




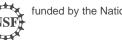




(Authenticate)

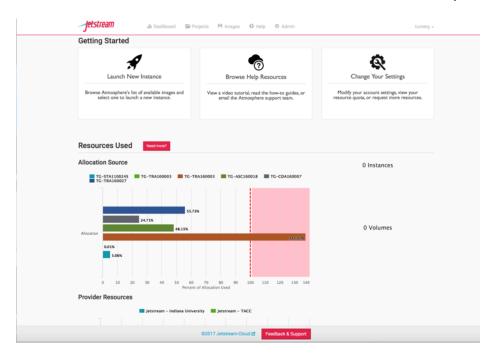








(user's home space)

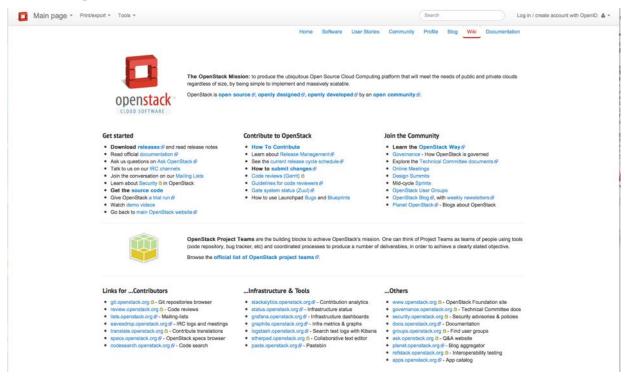








OpenStack Organization



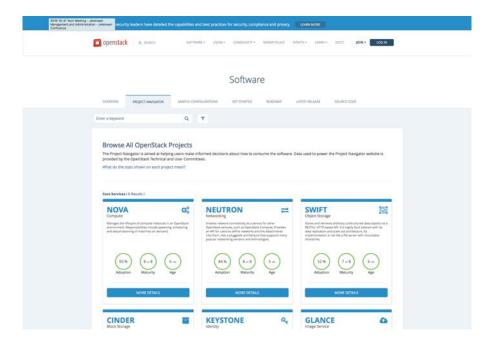








OpenStack Projects



http://www.openstack.org/software/project-navigator/





funded by the National Science Foundation

Award #ACI-1445604



Openstack Projects ...the core services

Service	Name	Adoption	Maturity	Age
Identity	Keystone	96%	7/8	5 yrs
Images	Glance	95%	6/8	7 yrs
Block device	Cinder	88%	7/8	5 yrs
Networking	Neutron	93%	7/8	5 yrs
Compute	Nova	95%	8/8	7 yrs
Object device	Swift	52%	7/8	7 yrs

https://www.openstack.org/software/project-navigator/





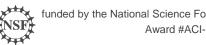


Openstack Projects ...some other services

Service	Name	Adoption	Maturity	Age
Dashboard	Horizon	87%	6/8	5 yrs
Telemetry	Ceilometer	55%	1/8	4 yrs
Database	Trove	13%	3/8	3 yrs
Orchestration	Heat	67%	6/8	4 yrs
Provisioning	Ironic	17%	2/8	3 yrs

https://www.openstack.org/software/project-navigator/





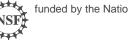


Openstack Projects ...some other services

Service	Name	Adoption	Maturity	Age
Map/Reduce	Sahara	10%	3/8	3 yrs
Shared Filesystems	Manila	14%	5/8	3 yrs
DNS Service	Designate	16%	3/8	3 yrs
Containers	Magnum	11%	2/8	2 yrs
Application Catalog	Murano	11%	1/8	2 yrs

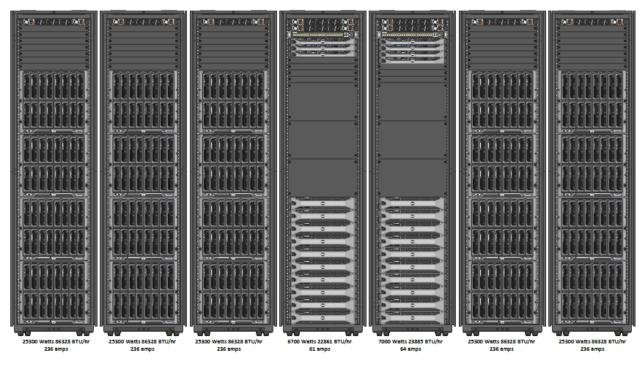
https://www.openstack.org/software/project-navigator/





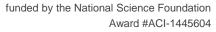


Jetstream Production Hardware











Just for fun: Happy Cluster – Mad Cluster





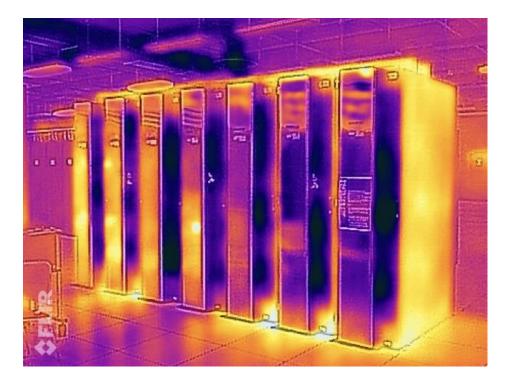








Infrared image of Jetstream

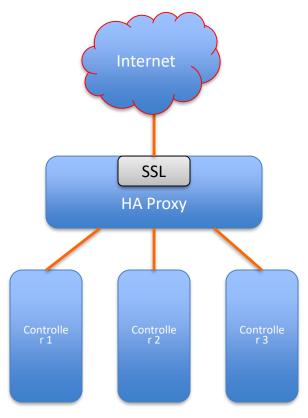


















Load Balancer 1



Load Balancer 2

Keep Alive

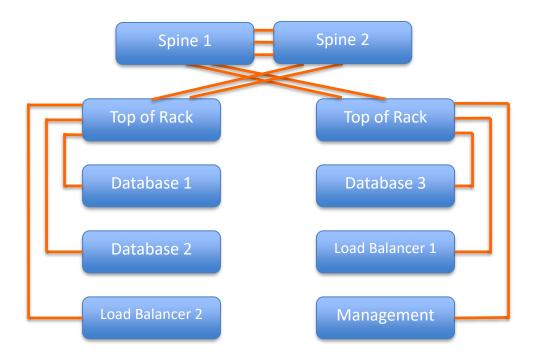
DNS Round Robin IP1 – IP2







High Availability layout for the databases

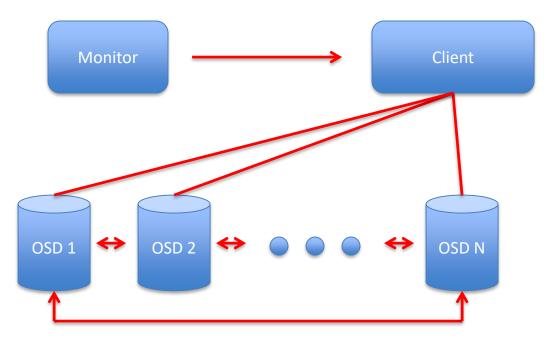








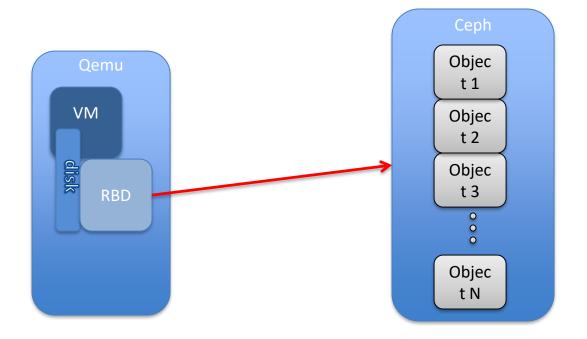
Glance - Cinder - Ceph



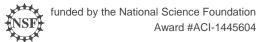






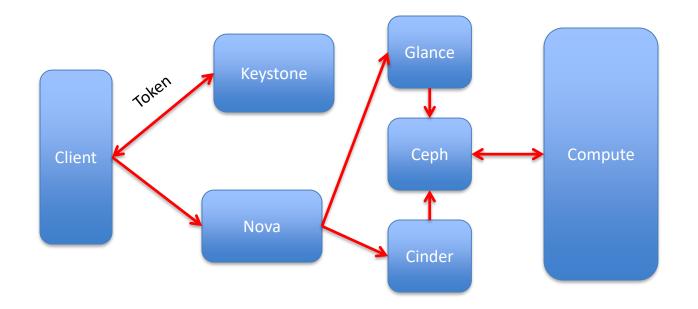




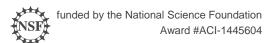




OpenStack Overview

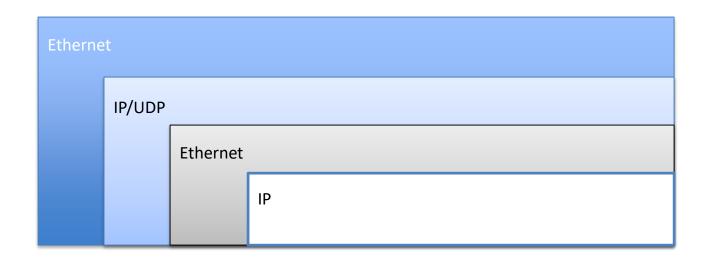




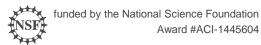




VXLAN Packet

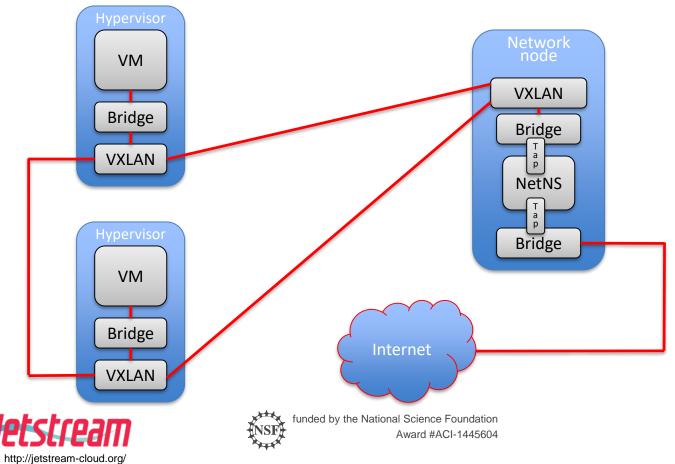








Neutron Networking



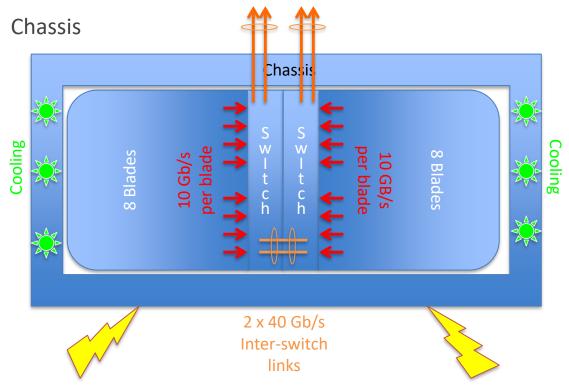


Network Topology (cont.)

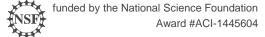
To Top of Rack Switches

Sixteen blades per chasses Two switches per chassis

10 Gb/s
40 Gb/s
LAG





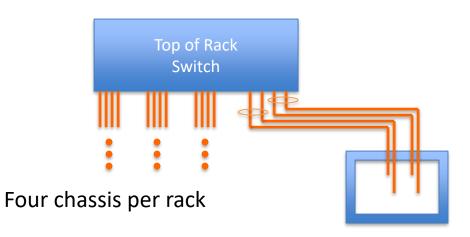




Network Topology (cont.)

Chassis to Top of Rack





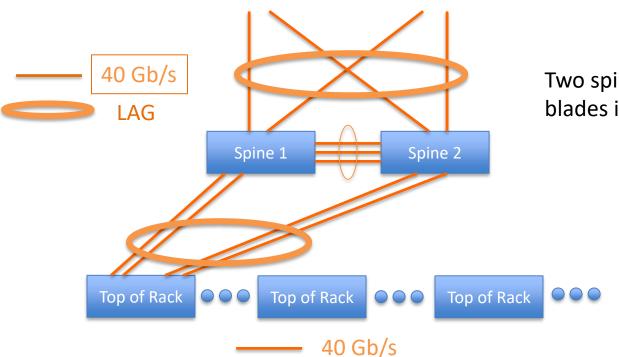
Two switches per chassis







Network Topology (cont.)



100 Gb/s uplink to Internet2

Two spines tie into two network blades in the datacenter switch

Seven racks tie into the two spine switches



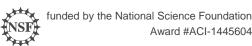




How do we onboard users onto Jetstream?

- An XSEDE User Portal (XUP) account is required. They are free!
 Get one at https://portal.xsede.org
- Read the Allocations Overview -<u>https://portal.xsede.org/allocations-overview</u>
- Write a successful allocation request start with a Startup or Education request - https://portal.xsede.org/successful-requests







Jetstream Information Sources

- Jetstream: https://use.jetstream-cloud.org/
- XSEDE User Portal is required to actually login: https://portal.xsede.org
- User guide: http://jetstream-cloud.org/training.php
- Paper describing Jetstream Jetstream: A self-provisioned, scalable scince and engineering cloud environment
- Configuration management: https://github.com/jetstream-cloud/Jetstream-Salt-States







Jetstream Partners



























Questions?

Project website: http://jetstream-cloud.org/

Project email: jethelp@iu.edu

Direct email: jomlowe@iu.edu, turnerg@iu.edu

License Terms

- Turner, G.. 2017. Jetstream, New Ventures in Research, Engineering and Educational Computing: Open Science Forum, Indiana University Bloomington, IN. Also available at: http://jetstream-cloud.org/publications.php
- Jetstream is supported by NSF award 1445604 (Craig Stewart, IU, PI)
- XSEDE is supported by NSF award 1053575 (John Towns, UIUC, PI)
- This research was supported in part by the Indiana University Pervasive Technology Institute, which was established with the assistance of a
 major award from the Lilly Endowment, Inc. Opinions presented here are those of the author(s) and do not necessarily represent the views of
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IVMOOC on Jetstream

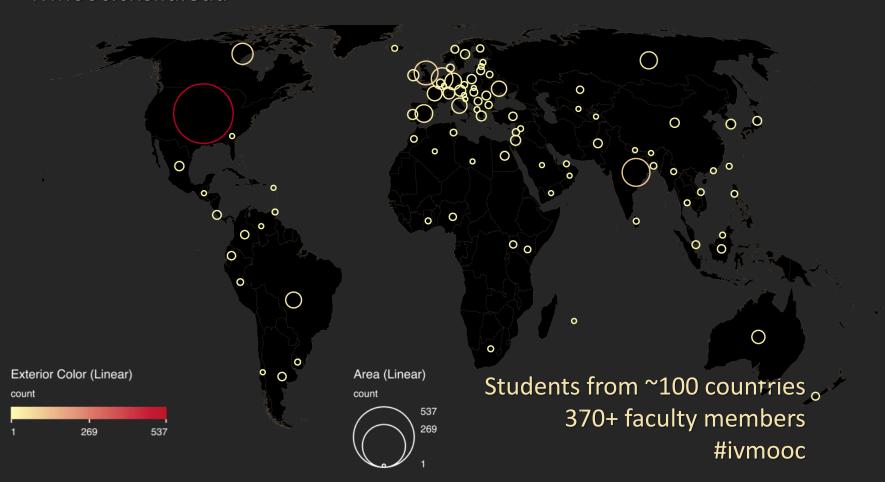
CNS, IUNI, UITS

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Register for free: http://ivmooc.cns.iu.edu. Class restarts Jan 09, 2018.

The Information Visualization MOOC ivmooc.cns.iu.edu



Part 1: Theory and Hands-On

Session 1 – Workflow Design and Visualization Framework

Session 2 – "When:" Temporal Data

Session 3 – "Where:" Geospatial Data

Session 4 – "What:" Topical Data

Mid-Term

Session 5 – "With Whom:" Trees

Session 6 – "With Whom:" Networks

Session 7 – Dynamic Visualizations and Deployment

Final Exam

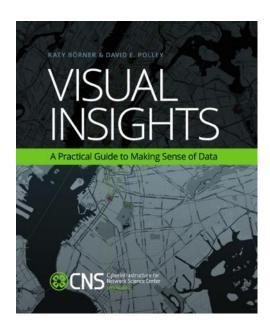
Part 2: Students work in teams on client projects.

Final grade is based on Class Participation (10%), Midterm (30%), Final Exam (30%), and Client Project(30%)



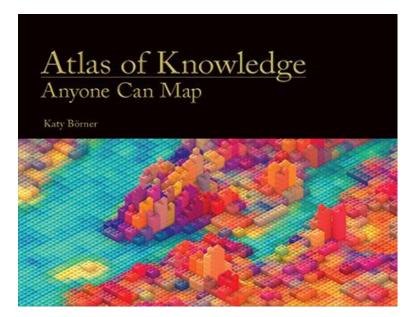


Books Used in the IVMOOC



Teaches timely knowledge:

Advanced algorithms, tools, and hands-on workflows.

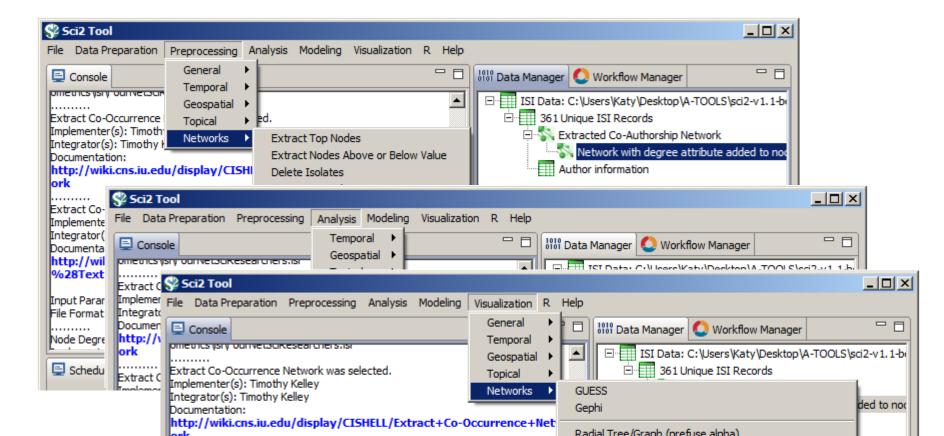


Teaches timeless knowledge:

Visualization framework—exemplified using generic visualization examples and pioneering visualizations.

Sci2 Tool Interface Components

Download tool for free at http://sci2.cns.iu.edu



IVMOOC 2017: Using NSF XSEDE and Jetstream to Run Data Analysis and Visualization Workflows in the Cloud

Katy Borner, 2017.04.20

In Spring 2017, IVMOOC students are invited to beta-test a novel cloud computing setup that supports low- to high-bandwidth users in running more compute intensive data analysis and visualization workflows in the cloud. Specifically, students will create a user account for the Extreme Science and Engineering Discovery Environment (XSEDE) and then use the Jetstream cloud-computing environment to run specific workflows using the Network Workbench Tool.



Hi students,

Best,

We wanted to let you know that there is a new assignment posted today that students can complete to earn an extra 2% to their final grade. (https://iu.instructure.com/courses/1595331/quizzes/2271360)

To earn the extra credit, students will have to create an account with XSEDE cloud computing program, and then run a compute instance on the Jet Stream platform to test running a workflow in the cloud environment.

To earn the extra credit, you will need to create your XSEDE account and submit your username to us by Monday April 24 at noon, then we'll link your account to Jetstream. Then from April 25-April 27th at noon, you will need to create an instance on the Jetstream, run a workflow, and submit your result to us.

Michael Katy and Andreas

Michael, Katy, and Andreas

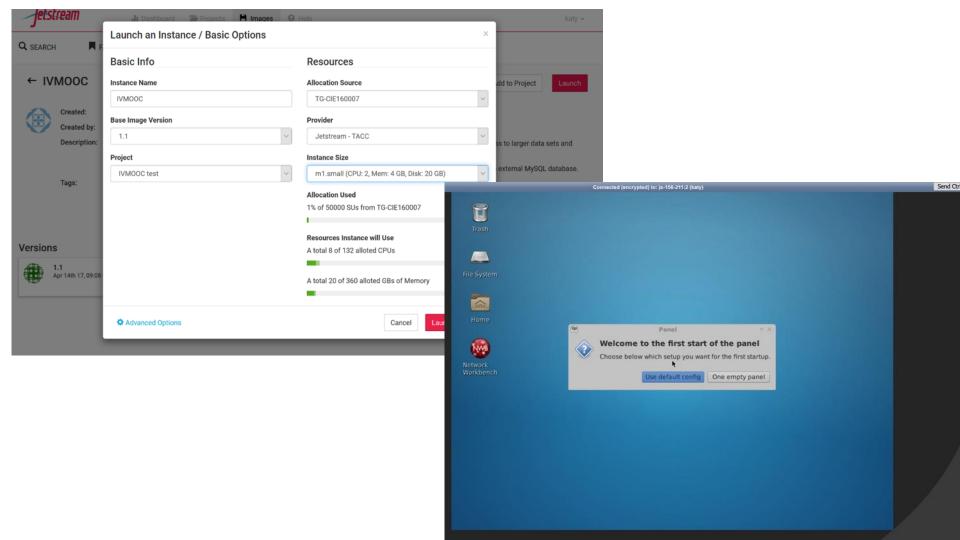
Account Setup

In order to use the IVMOOC Virtual Desktop via the Jetstream cloud environment, you need to get an XSEDE user account and this account needs to be linked to the IVMOOC cloud instance so that you can use this unique resource.

- Create an XSEDE user account via XSEDE User Portal.
- Submit your XSEDE user name via Canvas by 4/24, noon.
 (XSEDE user names were batch-added to IVMOOC VM)
- All IVMOOC students who submitted their XSEDE user name on time gained access to IVMOOC instance on Jetstream by 4/25.

Create to IVMOOC Instance on Jetstream

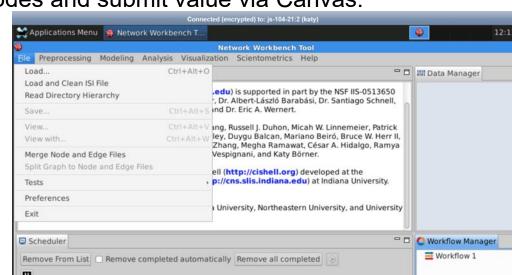
- After 4/25, noon, go to https://use.jetstream-cloud.org/application/images
- Login to use Jetstream using your existing organizational login, select "Indiana University" and use DUO.
- Select "Launch New Instance"
- Search for "IVMOOC" or directly go to https://use.jetstream-cloud.org/application/images/366
- Click on "Launch" in top right.
- Keep default values for the instance but increase "Instance Size" to m1.small (2 CPUs, 4096 GB memory, 20 GB disk). Click "Launch Instance" in lower right, see next slide.
- Wait until Status is "Active" then click on Instance with Name "IVMOOC."
- Wait until "Activity" is N/A (about 1-2 mins). The VW is now ready for usage.
- Reload page. "Open Web Desktop" should now be visible in lower right. Click on it to open virtual desktop in web browser.
- Confirm "Use default config."



Run NWB Tool

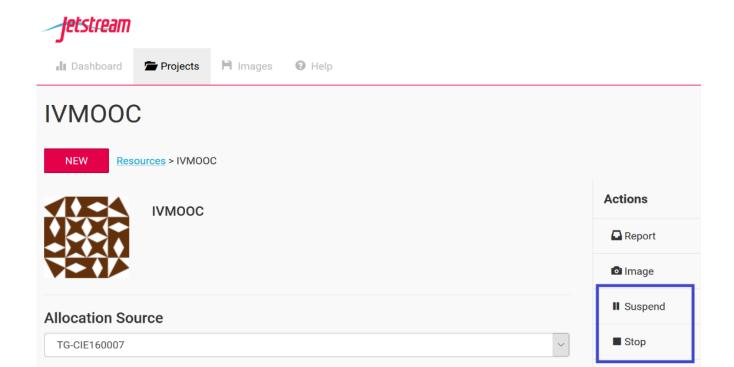
- On Web Desktop, double click Network Workbench (NWB) to run the tool.
- Run "Model > Hypergrid" and generate a network with 10,000 nodes and a Maximum degree of each node: 4.
- With the Hypergrid Network Model being selected in the Data Manager, run "Analysis > Network Analysis Toolkit (NAT)."
- Record the "Average degree" for nodes and submit value via Canvas.
- Feel free to try out other workflows.

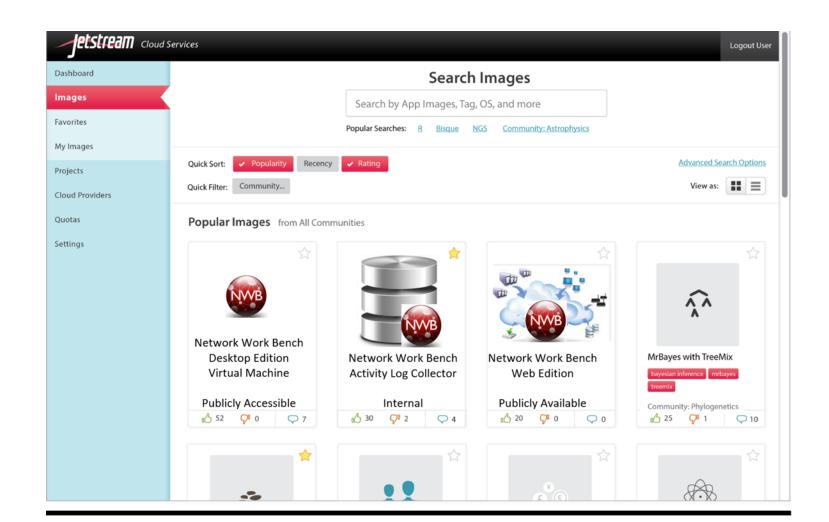
Fletcher, George, Hardik Sheth, and Katy Börner. 2005. "Unstructured Peer-to-Peer Networks: Topological Properties and Search Performance". Agents and Peer-to-Peer Computing: Third International Workshop, AP2PC 2004. New York, NY 14-27

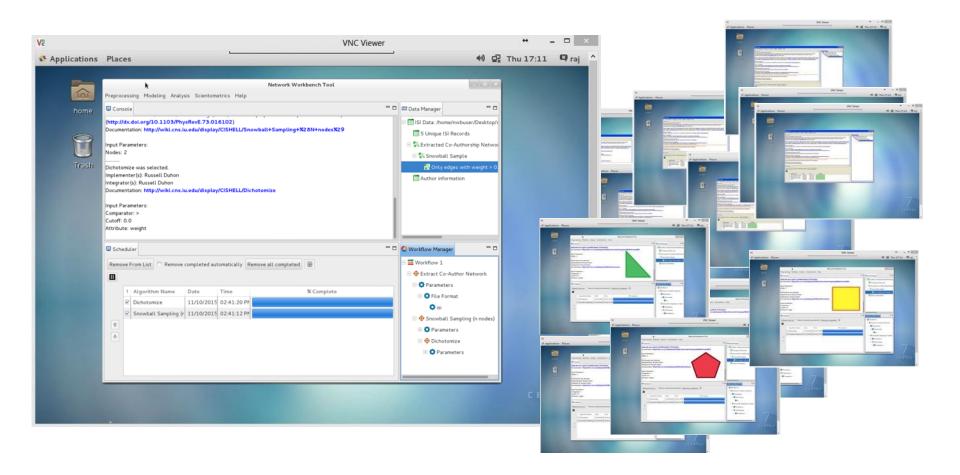


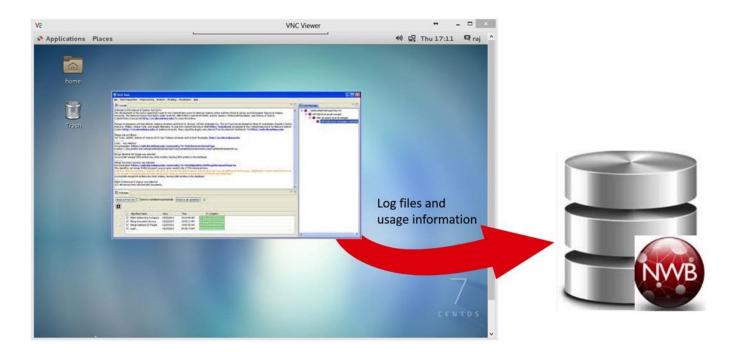
Suspend/Stop IVMOOC Instance on Jetstream

When done, go back to Jetstream web interface and click on "Suspend" or "Stop" in Actions list on right:









- Logging allows for capturing all user actions.
- Supports student evaluation and guidance.
- Helps identify frequency of dataset/algorithm usage per branch of science in support of future tool development.





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Open XD Metrics on Demand Value Analytics

CNS, IUNI, UITS

INDIANA UNIVERSITY BLOOMINGTON







Supported by the National Science Foundation

Matt Link

Associate Vice President (Acting)

Director, Systems

Research Technologies, Pervasive Technology Institute

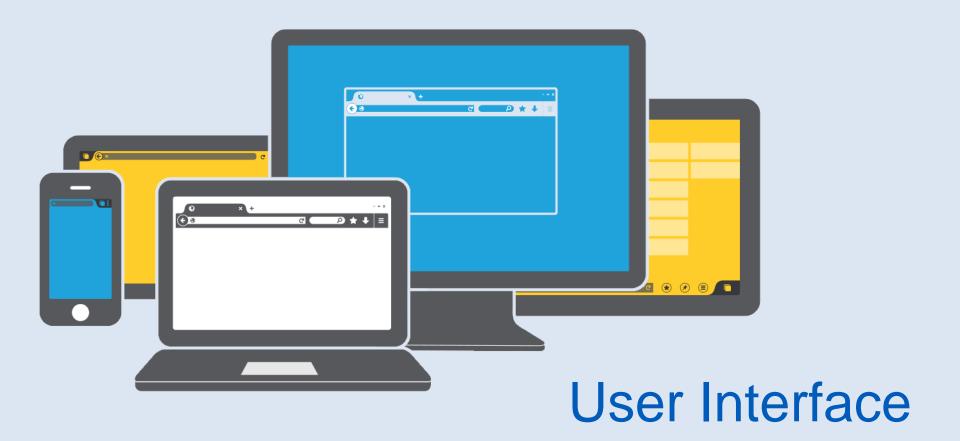
Office of the Vice President for IT, Indiana University



- Developed by the University at Buffalo Center for Computational Research
- Comprehensive resource management for HPC systems
- Provide detailed operational and usage data
- Support optimization of HPC resource utilization
- Facilitate planning and analysis
- Used for XSEDE metrics

XDMoD – Value Analytics

- NSF eager award to Indiana University and University at Buffalo
- Collaboration between the Center for Computational Research at the University at Buffalo, and the Pervasive Technology Institute and Center for Network Science at Indiana University
- Enables academic institutions to better understand Return
 On Investment (ROI) on advanced Cyberinfrastructure (CI)
- Shows the value of:
 - Fostering collaboration
 - Supporting scientific publications
 - Show relationship between campus CI and external grant funding
- Local XDMoD installation required all data kept locally²



VA module will be integrated into local¹





Grant data

Why it's important

"Since Big Red's installation in 2006, users of that system were PIs or project directors on a total of \$253 million in external funding, which includes \$65.4M in facilities and administration funds. In addition to the research dollars flowing into the University, the ability to leverage IU's leadership in research cyberinfrastructure has aided many other grants awarded to IU."

-2010

PTI: Funding analytics

HPC and Biomedical Usage...

No use of Research CI 39%

Biomedical Software Usage 25%

HPC Facility Usage 18%

Screen shots of PTI developed statistics tool.

RT Stats

Biochemistry/Molecular Biology (Indianapolis)

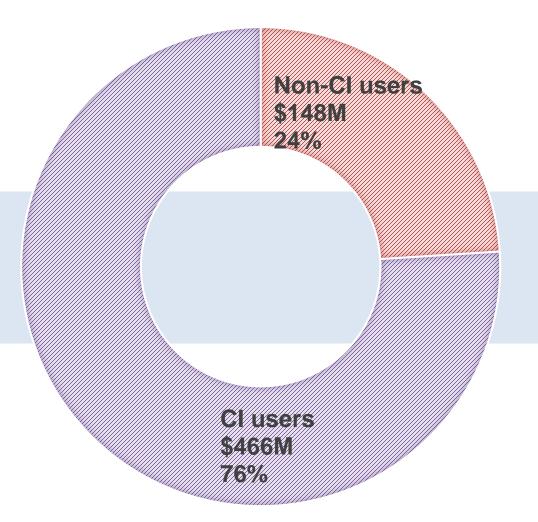
School Of Medicine

Biochem Auxiliary Bioinformatics Biom Chemical Genomics Diabetes Basic Science Res Services Program Ctr Abdul Sater, Zahi A Arthur, Jack W Cerabona, Donna Conteh, Abass Craven, Kelly Edenberg, Howard J Folck, Anthony F Fox. Melanie J Gendron, Jaimie M Fusakio, Michael Georgiadis, Millie M Heyen, Joshua W Heyerdahl, Darcy Hoang, Ouven O Huang, Fei Hunter, Gerald O

Grants24 totaling \$6,056,352.00

Grant	Project	Status	Dates	Award Total
043956-00005B	Docking uPAR for Selective Targeting of Cancer Metastasis	New	January 2015 - June 2016	\$180,000.00
044265-00004B	The Bipolar Genome Study	New	May 2014 - April 2016	\$87,728.00
053198-00014B	Collaborative Study on the Genetics of Alcoholism (COGA)	New	September 2015 – August 2016	\$1,480,906.00
054541-00005B	Regulation of RNA Polymerase II Transcription by the Phosphatase Rtr1	New	August 2015 - July 2016	\$291,461.00
054541-00007B	Regulation of RNA Polymerase II transcription by the phosphatase Rtr1	New	August 2015 - July 2016	\$34,710.00
056553-00006B	Non-Homologous End Joining Repair in Human	New	April 2015 - March 2016	\$319,550.00
056564-00005B	Metabolic stress resones and EIF2 kinase GCN2	New	May 2014 - April 2016	\$343,929.00
056564-00008B	Metabolic stress responses and eIF2 kinase GCN2	New	May 2014 - May 2016	\$116,099.00
057512-00006B	Early binge drinking and gene regulation	New	September 2015 – August 2016	\$225,424.00

2016 IU grant income **\$614M**



Grant data capabilities

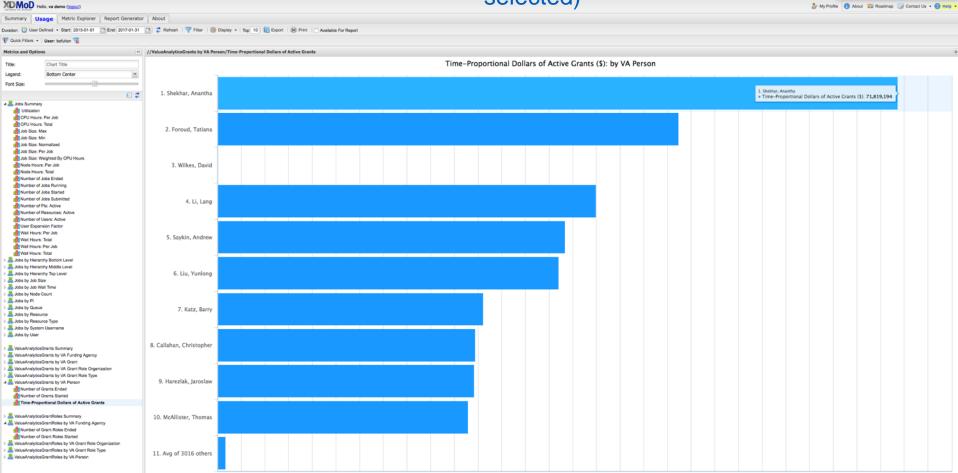
Current

- IU KFS export -> JSON convert -> XDMoD_VA ingest
- NIH and NSF from public datasets
 - IU to provide scripts for NIH and NSF data imports to local³ XDMoD_VA instance

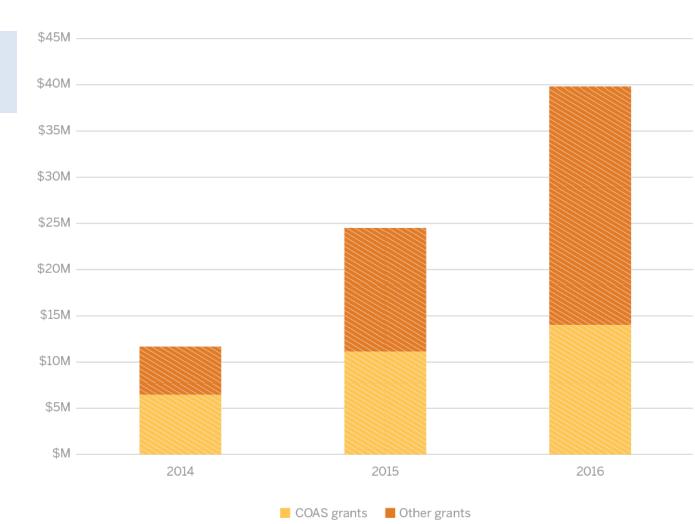
Future

Ability to group by organizational structure(as seen in PTI slide) (IMS export)

Grant dollars per PI (based on timeline selected)

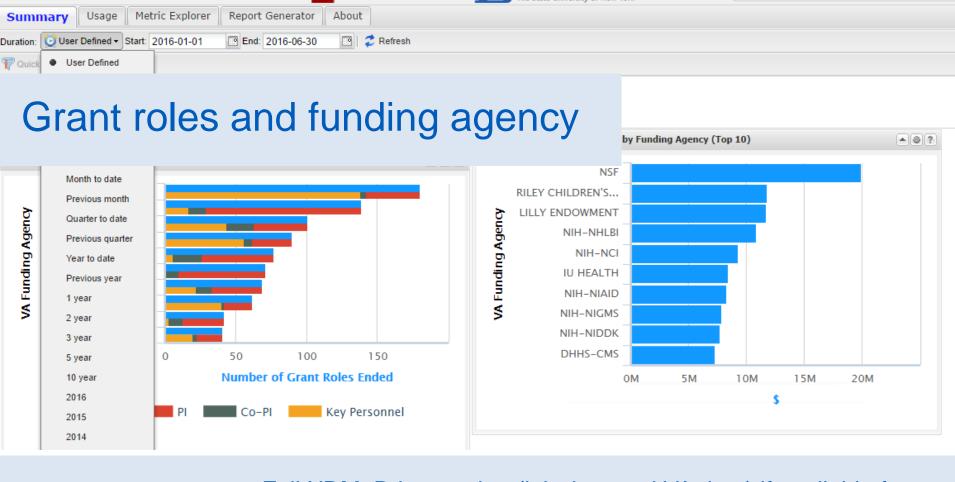


Future capability (grouped by organizational structure)



Roles and funding





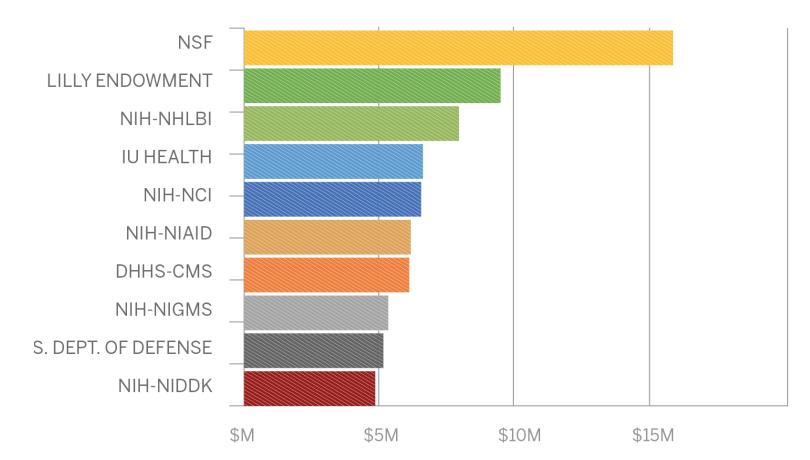
INDIANA UNIVERSITY

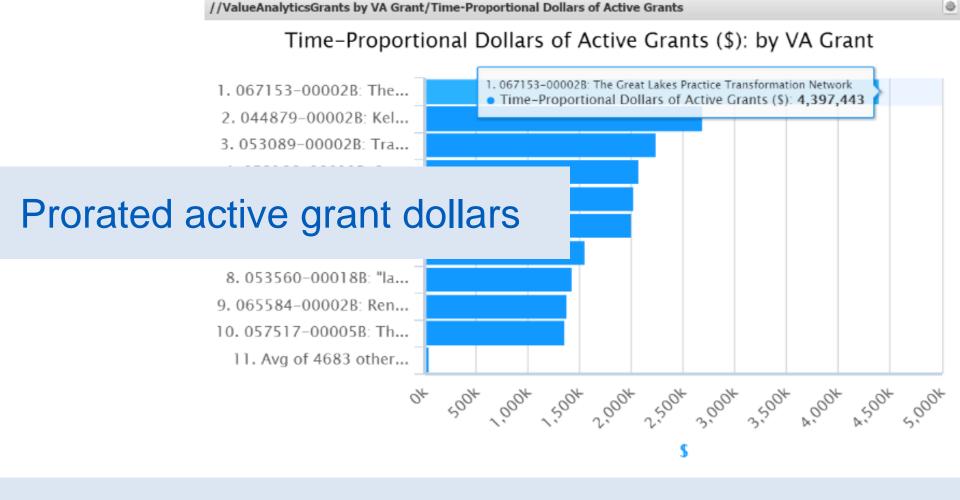
XDMOD Hello, Value Analytics Demo (loqout)

Full XDMoD integration (job data and VA data) if available from

University at Buffalo My Profile About Roadmap Contact Us + Photography Help To Profile About Roadmap

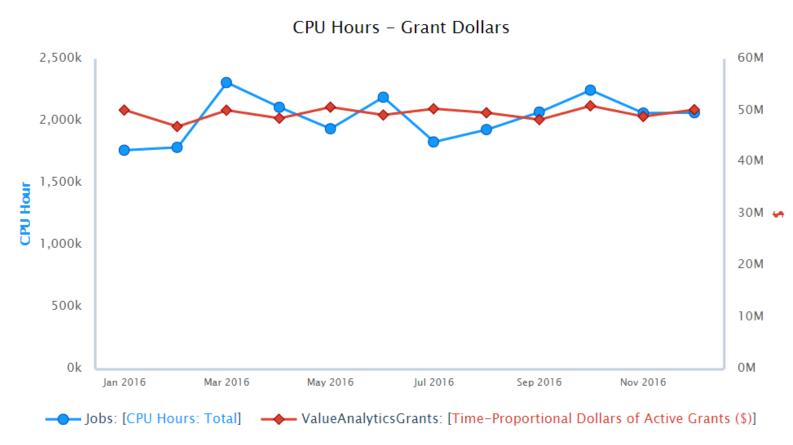
Grant dollars by funding agency

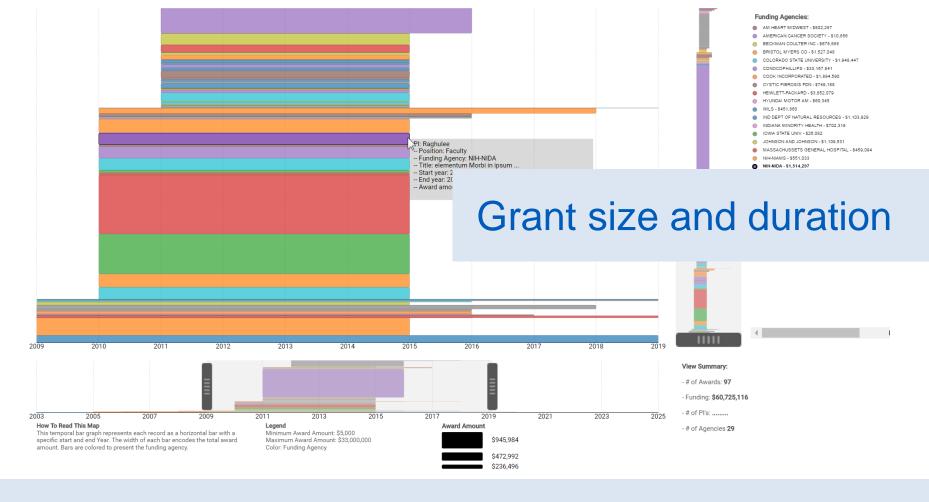




Ability to drill down to individual grants

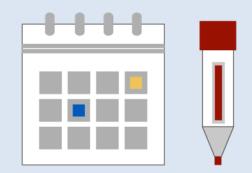
Combined HPC job statistics and value analytics metrics





Grants over time associated with funding





Publication data





Publication data capabilities

Current

- Working to develop XDMoD schema for ingest
- Access to NIH grant and publication data available
 - NIH Exporter (https://exporter.nih.gov/)
 - Limited visualization capabilities

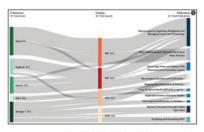
Future

- Roadmap to link publication and grant data
- Ability to group by organizational structure
- Visualization capabilities integrated

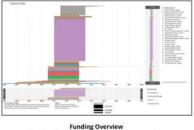
XDMOD Value Analytics



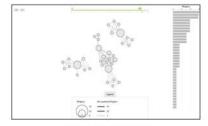
Value Analytics



Funding and Publication Impact Impact of IT resources on external funding and publications.

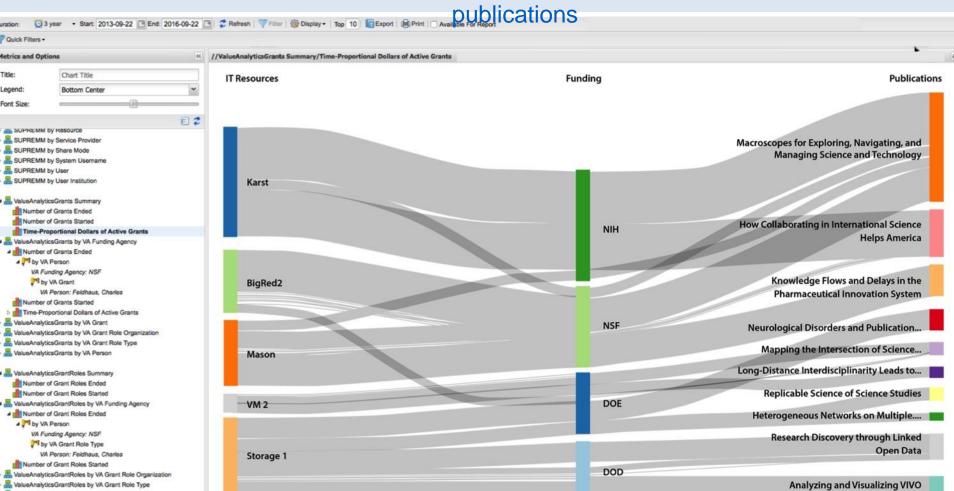


Funding Overview
Funding duration, amounts, and types over time.



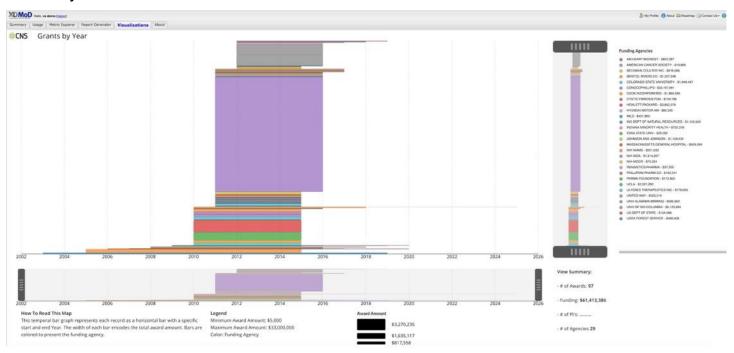
Co-PI Collaboration Network
Co-PI collaboration network based on NSF funding data.

Integrated view: CI resources, funding, and

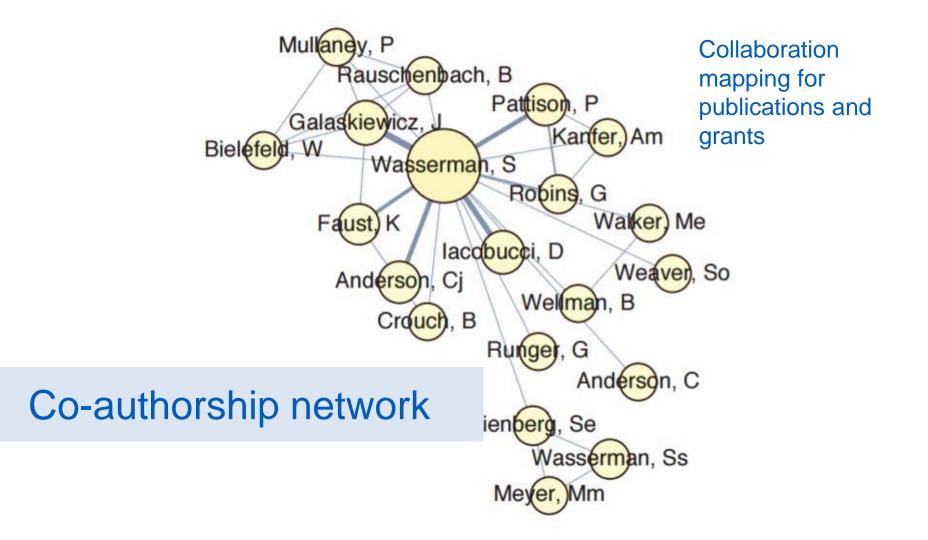


Visualization: Temporal Bar Graph

Project: XDMoD



This temporal bar graph represents each record as a horizontal bar with a specific start and end year. The width of each bar encodes the total award amount. Bars are colored to represent the funding agency (legend of funding agencies are listed on the right). This graph shows funding duration, amounts, and types over time.

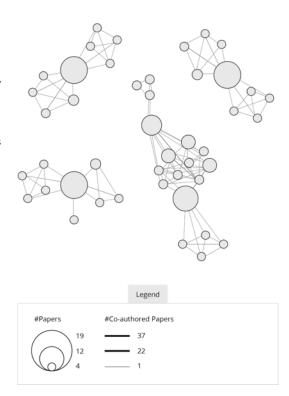


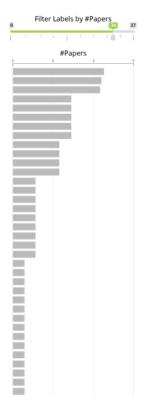
Visualization: Co-PI Network

Project: XDMoD

+ -

This network represents collaboration patterns based on NSF funding data. Each node represents a principal investigator (PI or Co-PI). It is labelled by the PI's name, size coded by the total value of all awards for each PI, and color coded by the number of collaborators. An edge between two PIs denotes that they have a grant together with edge thickness denoting the number of times they collaborated and edge color reflecting their success in terms of total sum of all their joint awards. The listing on right rank orders PIs by total dollar amounts.





XDMoD Roadmap



June 2017

Cross-Referencing Grants and HPC Usage Data

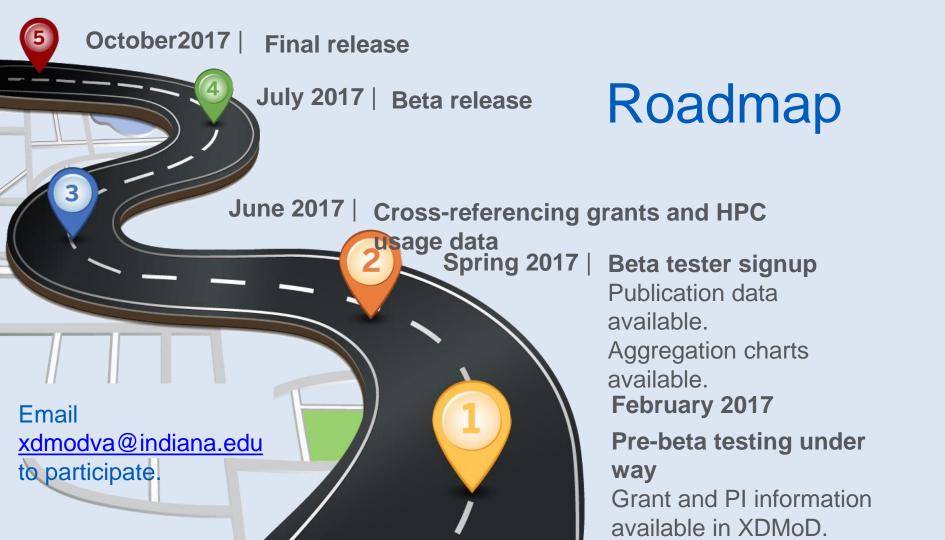
Spring 2017

Beta tester signup
Publication data available
Aggregation charts available

February 2017

Pre-Beta Testing Under Way

Grants and PI information available in XDMoD



Beta program requirements

- Install and maintain Open XDMoD local⁴ instance
- Ability to ingest job logs from computational systems
- Ability to get your grant data from your Office of Research Administration
 - We will help you write a script to convert your data to JSON format for ingestion
- Engagement from your institution (you, ORA)
- Rice and SDSC are our two beta testers so far
- Several institutions expressed interest we'll be in touch

Thank you.⁵ Questions?

Contact: xdmodva@indiana.edu

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