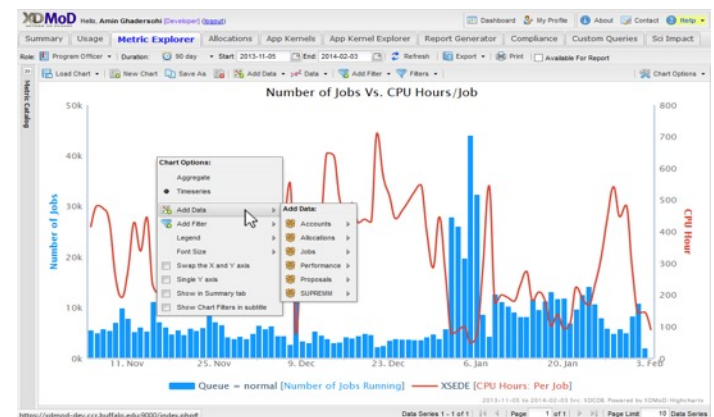
A photograph of a server room with blue lighting. Two people are standing in the aisle, talking. The text is overlaid on the image.

ACCESS Monitoring and Measurement Service (MMS) Overview SURA - June 2022

ACCESS MMS Team

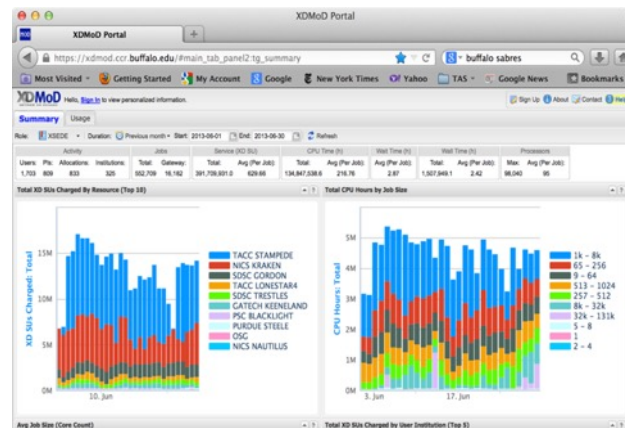
Outline

- **ACCESS Monitoring and Measurement Service (MMS)**
 - ACCESS MMS Team
- **Why a CI Monitoring and Measurement Service?**
 - Potential for High Impact
 - Stakeholder Benefits
 - Data/Services Available to ACCESS Tracks
- **ACCESS MMS – What’s New**
 - Data Analytics Framework
 - CI Simulator
 - Monitoring CI Ecosystem
 - Application Power Monitoring
 - Network Integration
 - Value Analytics Realm
 - Open XDMoD Development
 - ACCESS Auditing
 - Service Model
- **Discussion**



ACCESS Monitoring and Measurement Service

- **Comprehensive framework for CI system management**
- **Understand and optimize resource utilization and performance**
 - Provide instantaneous and historical information on utilization
 - Measure Quality of Service of CI systems and applications
 - Measure and improve job and system level performance
 - Inform computing system upgrades and procurements
- **XDMoD (XD Metrics on Demand) tool**
 - Analytics Framework for XSEDE/ACCESS
- **Open XDMoD*: Open Source version for CI centers**
 - Used to measure and optimize performance of HPC centers
 - 250+ academic, governmental, & commercial installations worldwide
 - <https://open.xdmod.org/>



ACCESS MMS Team

- **University at Buffalo – Center for Computational Research**
 - Matt Jones, Bob DeLeon, Joe White, Jeff Palmer, Nikolay Simakov, Ryan Rathsam, Gregory Dean, Hannah Taylor, Conner Saeli
- **Roswell Park**
 - Tom Furlani (PI)
- **TACC**
 - Bill Barth, Stephen Harrell, Matt Cawood (performance monitoring)
- **Tufts**
 - Abani Patra (performance monitoring)
- **Indiana**
 - Jennifer Schopf (Netsage)
- **Case Western**
 - Vipin Chaudhary (application anomaly detection)
- **SDSC**
 - Shava Smallen (CloudBank)



Why a CI Monitoring and Measurement Service?

- **Monitoring and Audit of NSF funded CI**
 - Technology Audit Service (TAS): 2010 – 2015
 - XD Metrics Service (XMS): 2015 – 2022
- **The landscape before TAS/XMS**
 - Accounting data incomplete and only available quarterly
 - Job level performance data not available
 - No external measure of Quality of Service (QoS)
 - RP reporting to the central database was inconsistent
 - RP quarterly and annual reports done manually
 - CI planning and analysis difficult due to lack of accessibility of historical data (utilization, allocation, etc)



Overall CI Performance Matters

- **CI systems are typically oversubscribed**
 - Improving application or system performance will improve overall job throughput
 - Free's up otherwise wasted CPU cycles for useful work
- **Small improvements in system performance can have high impact**
 - Every 1% increase in system performance on the resources provided through XSEDE translates into the ability to allocate an additional 101 M CPU hours annually
 - Corresponds to a savings of \$5M*

* Assuming a rate of \$0.05 per CPU hour



Benefits for Stakeholders

- **PI and End User**
 - Account management, resource selection, application tuning, improved throughput
- **Systems Administrator**
 - System diagnostic and performance optimization, application tuning
- **Computational Scientist and Support Specialist**
 - Tool to facilitate work with end-users to improve job performance and throughput
- **CI Center Director**
 - Comprehensive resource management and planning tool
 - Return on Investment Metrics
- **External Reviewers**
 - Tool for data driven review for verification of best practices and project goals
- **NSF Senior Leadership**
 - Measure the effectiveness of supported programs
 - Inform deployment of future systems to fulfill unmet need



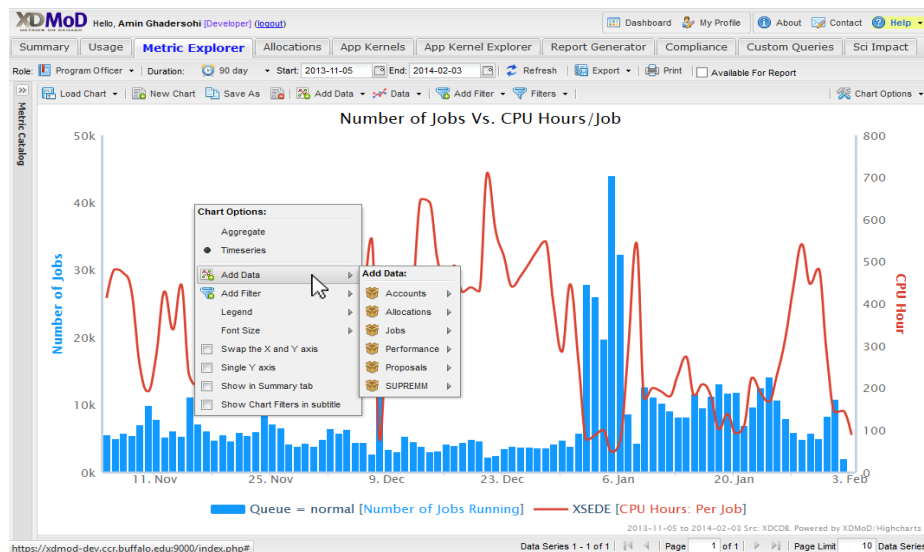
Data/Services Available to ACCESS Tracks

- Job accounting data
- Application performance data
- Allocations data
 - Users, Resources
- Gateways usage data
- Quality of Service data
 - Resource providers
 - Applications
- Job efficiency data
- User data
 - Job efficiency, usage, application performance,
- Resource workload analysis
- Data analytics framework
- Networking data
- Workflows



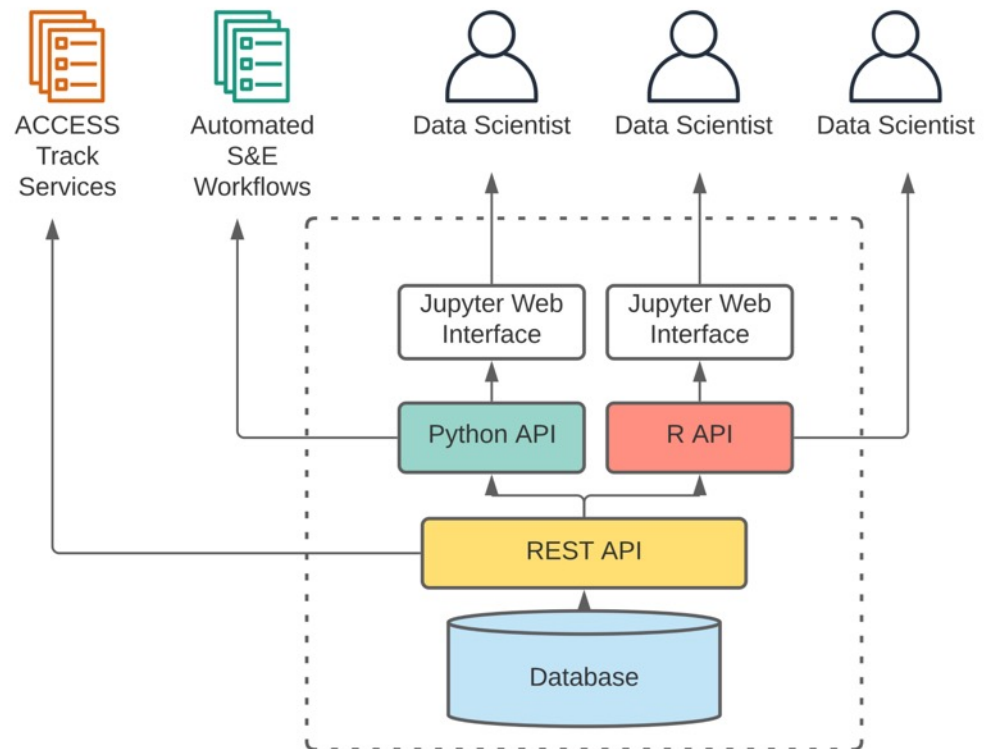
So What's New?

- **ACCESS MMS Tasks**
 - Data Analytics Framework
 - CI Simulator
 - Monitoring CI Ecosystem
 - Application Power Monitoring
 - Network Integration
 - Value Analytics Realm
 - Open XDMoD Development
 - ACCESS Auditing
 - Service Model

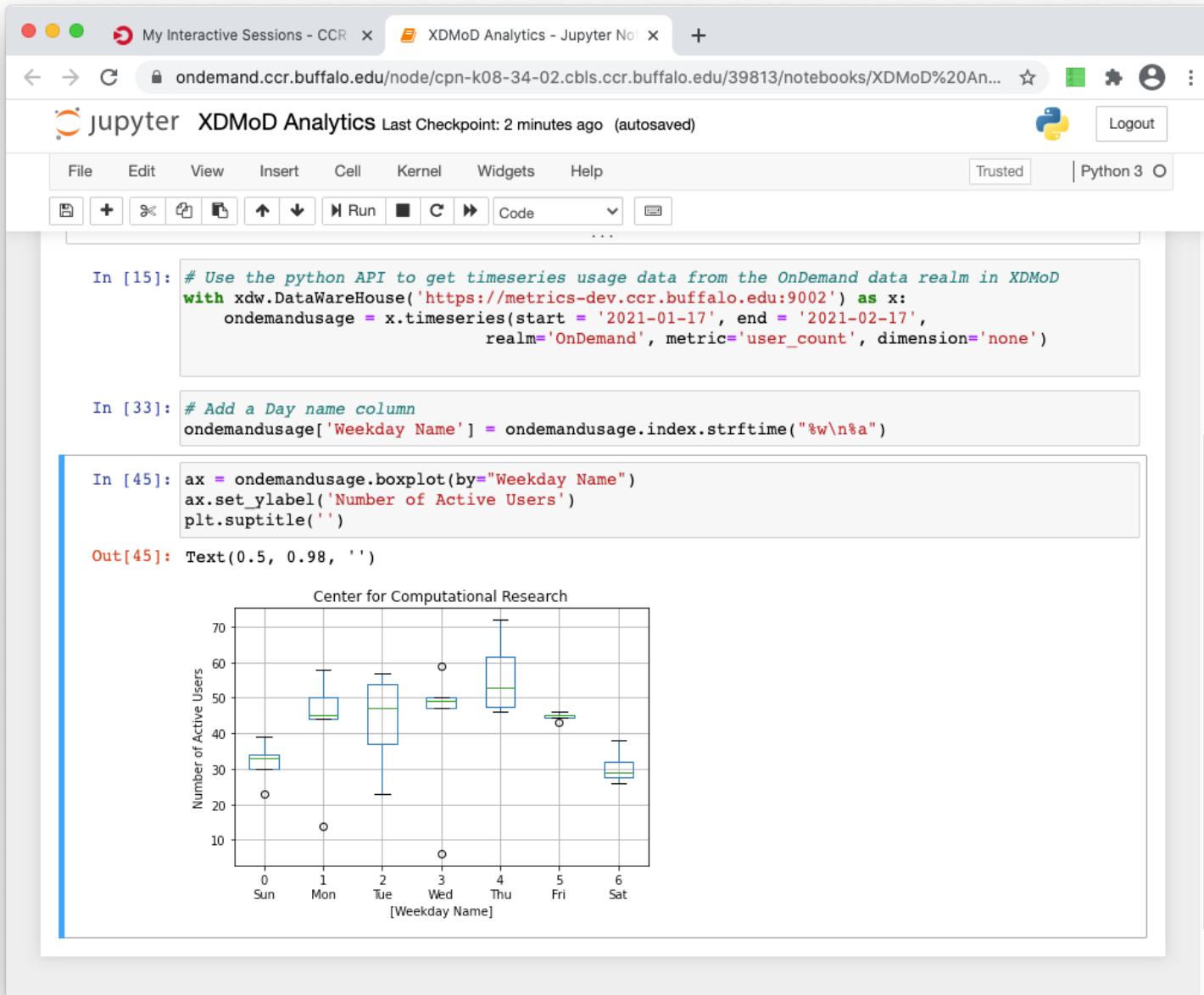


Data Analytics Framework

- Provide analytic framework for direct access to rich depository of performance and utilization data in XDMoD data warehouse
- No reliance on XDMoD web portal
- GUI Built on Jupyter notebooks
- Python and R interfaces for automated workflows and expert users



Data Analytics Framework Prototype



The screenshot shows a Jupyter Notebook interface with the following content:

```
In [15]: # Use the python API to get timeseries usage data from the OnDemand data realm in XDMoD
with xdw.DataWarehouse('https://metrics-dev.ccr.buffalo.edu:9002') as x:
    ondemandusage = x.timeseries(start = '2021-01-17', end = '2021-02-17',
                                  realm='OnDemand', metric='user_count', dimension='none')
```

```
In [33]: # Add a Day name column
ondemandusage['Weekday Name'] = ondemandusage.index.strftime("%w\n%a")
```

```
In [45]: ax = ondemandusage.boxplot(by="Weekday Name")
ax.set_ylabel('Number of Active Users')
plt.suptitle('')
```

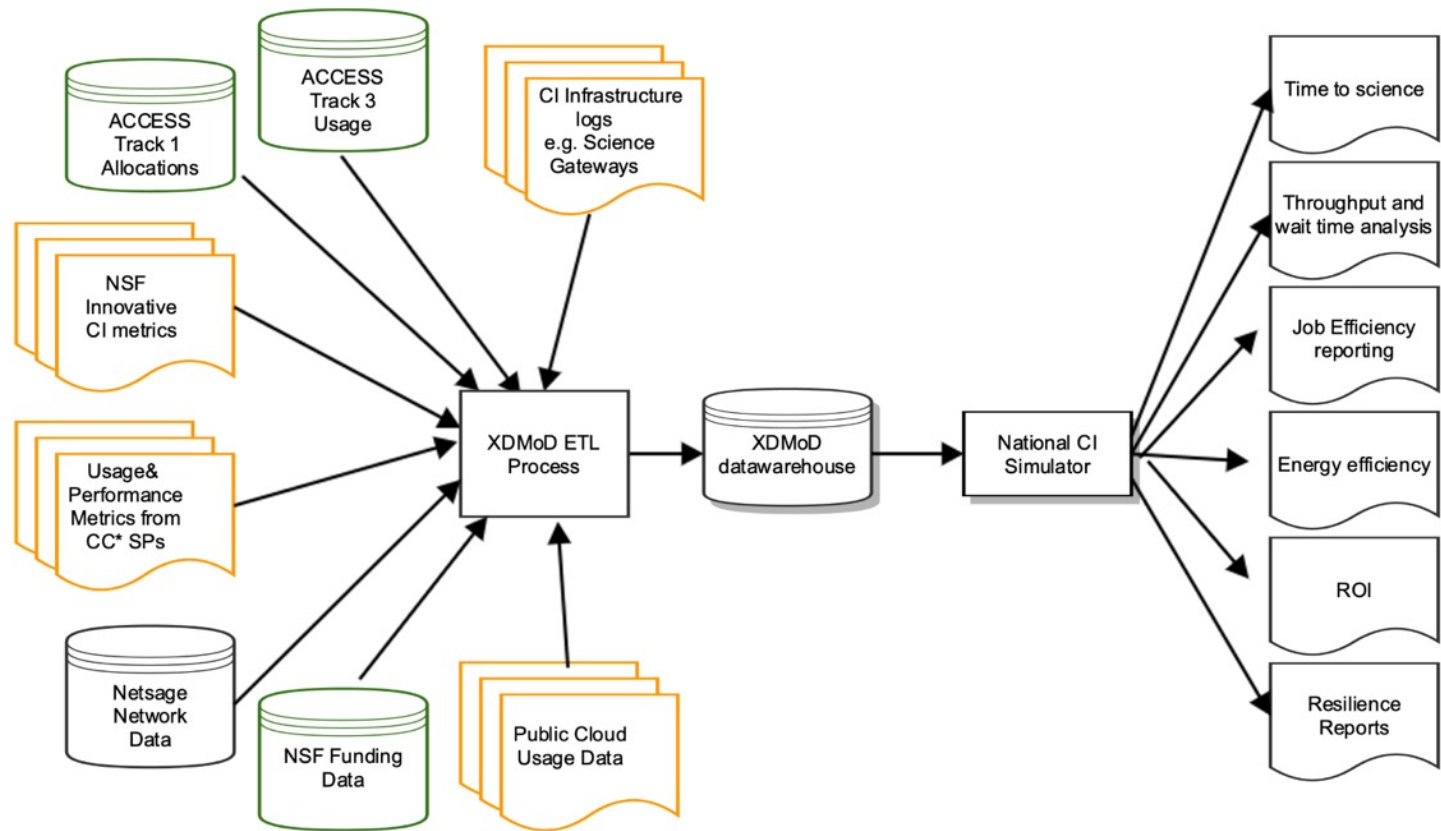
Out[45]: Text(0.5, 0.98, '')

The visualization is a box plot titled "Center for Computational Research". The y-axis is labeled "Number of Active Users" and ranges from 0 to 70. The x-axis is labeled "[Weekday Name]" and shows days 0 through 6 (Sun through Sat). The plot shows the distribution of active users for each day, with Thursday having the highest median and Friday having the lowest.

Weekday Name	Min	Q1	Median	Q3	Max	Outliers
Sun	20	30	32	35	40	25
Mon	15	45	48	50	58	15
Tue	25	38	48	55	58	25
Wed	5	48	49	50	50	5, 60
Thu	45	48	52	62	70	45
Fri	42	43	44	45	46	43
Sat	25	28	29	32	38	25

CI Simulator

- **Develop a CI Simulator to model the NSF CI ecosystem**
- **Can be used to predict the response CI ecosystem to:**
 - New CI systems
 - Changes in the operational parameters of existing systems



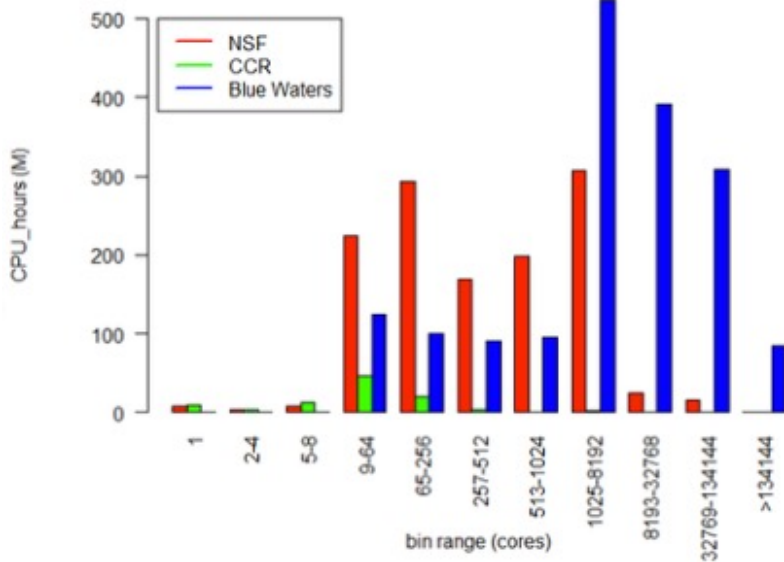
CI Simulator

- **Specific questions can be posed and the CI simulator can provide a quantitative estimate of response of CI ecosystem**
- **Example use cases**
 - Which of the following options would have the greatest impact on reducing the time to science:
 - one large resource,
 - two smaller resources,
 - or additional public cloud resources?
 - Simulating the relative impact of increased gateway resources versus MRI or CC* resources, which can then be used to guide funding decisions.



Monitoring the CI Ecosystem

- Current XDMoD monitoring framework employed to better understand national capacity and capability class CI systems
- However, this represents a continually shrinking fraction of the national computational CI ecosystem which includes:
 - campus-based systems, high throughput computing, science gateways, and public clouds



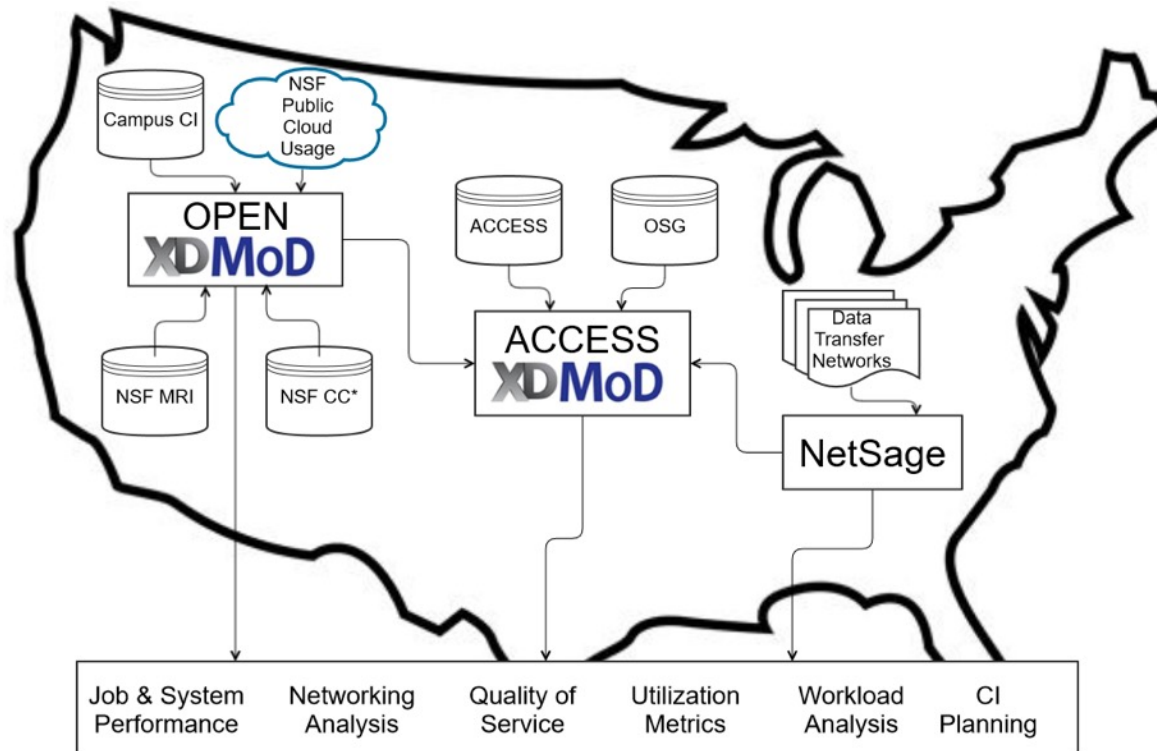
a



b

Monitoring CI Ecosystem

- Development of a monitoring system for CI computational ecosystem
 - national-level CI
 - NSF-funded public cloud usage
 - campus-level CI
 - network utilization
 - workload-type systems (OSG and Gateways)



NSF National Computational CI

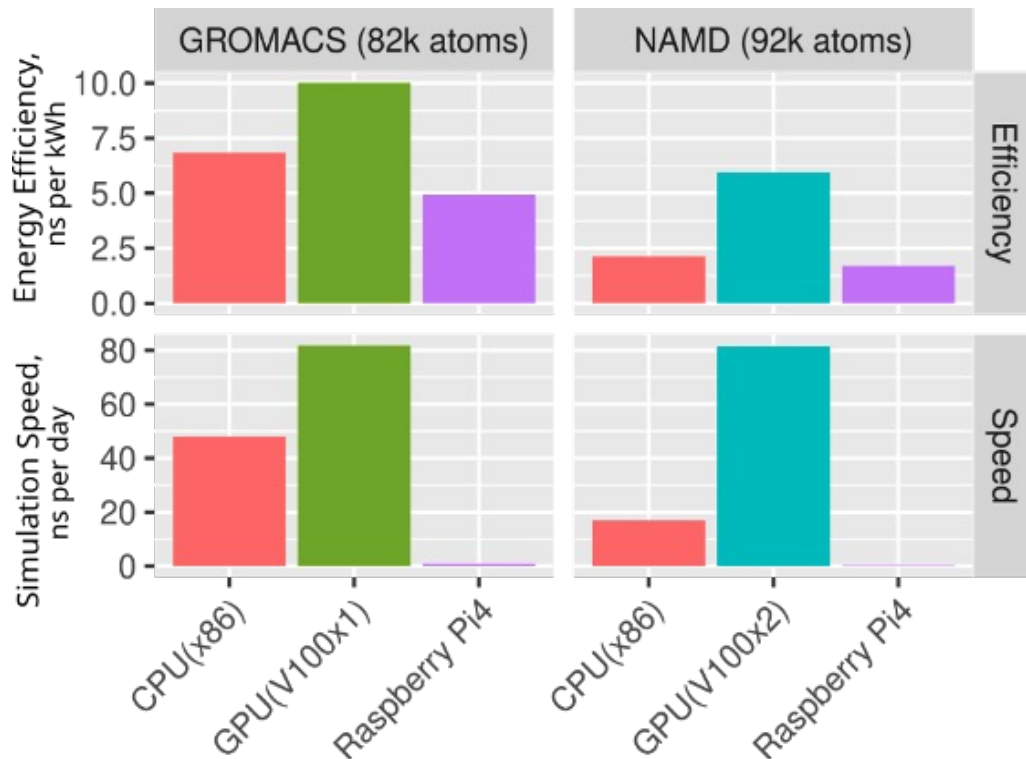
Application-Level Power Monitoring

- **Provide a detailed workload analysis of time to solution versus power consumed for applications**
- **Useful for new and emerging technologies**
 - Will the energy savings realized by a more energy efficient architecture be offset by longer running times for the job mix?
- **Application developers can tune their applications to achieve better energy efficiency on different architectures**



Application-Level Power Monitoring

- **Example: Energy efficiency comparison for NAMD and GROMACS**
 - CPU - Intel Gold-6230,
 - GPU-NVIDIA V100
 - Raspberry Pi4 (ARM-based)



GPU versions are faster and more energy efficient

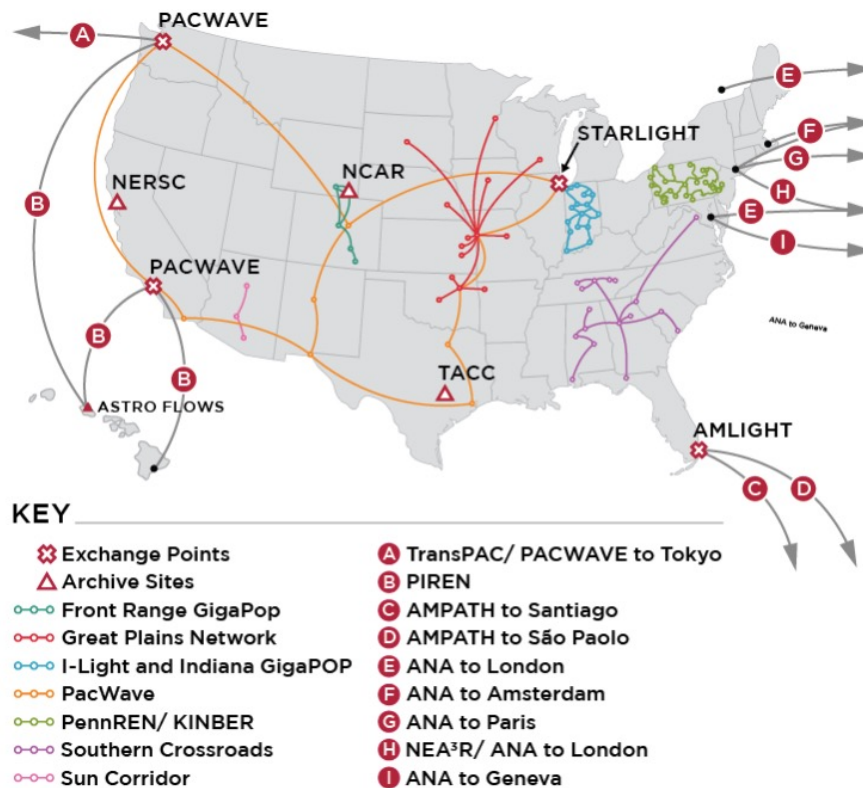
Application Performance Diagnostics (Case Western Reserve University)

- **Effective application monitoring requires full stack monitoring from the front-end, user experience, to the back-end CI to provide complete visibility into every aspect of application performance**
 - Various layers such as infrastructure, network, logs, containers, databases, and clouds.
- **Develop machine learning based tools to monitor application performance metrics**
 - Develop framework with lightweight agents for real-time
 - Train models using time-series data from XDMoD
 - Target two widely used applications



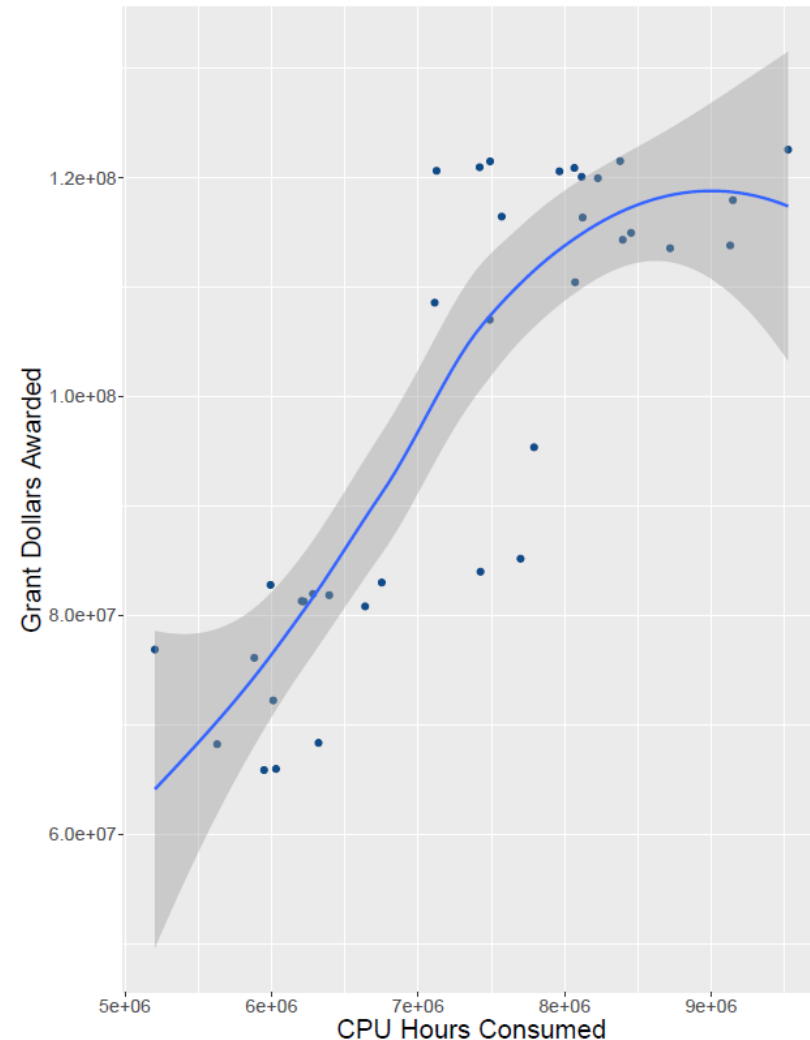
Network Data Integration

- Indiana University – Dr. Jennifer Schopf
- Motivation: Data movement increasingly important for computation, simulation and large-scale experimental facilities
- Use NetSage to track data movement
 - Collect SNMP, flow data, and perfSONAR active testing data
- Use XDMoD to correlate data movement with computational workload



Value Analytics Realm in XDMoD

- Help provide ROI metrics to support campus investment in CI
- XDMoD Value Analytics Realm will correlate system usage with PI funding
- Proposed sources of campus funding data
 - university sponsored programs office
 - direct feeds from NIH, NSF, etc



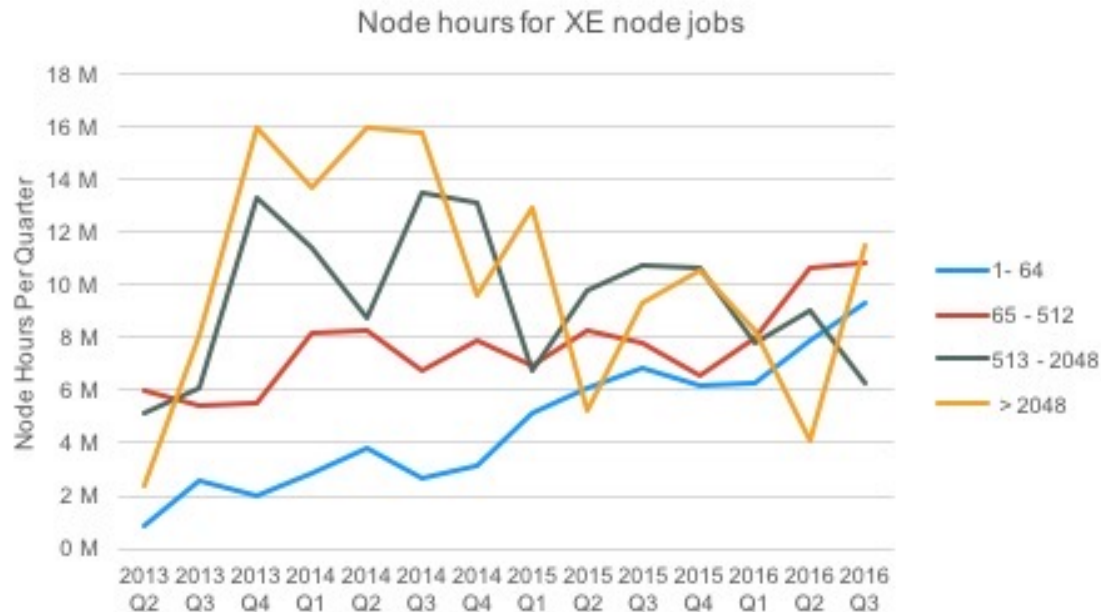
XDMoD & Open XDMoD Development

- **TACC_Stats development**
 - keep current, add new technologies and new features
- **Additional features including:**
 - Added GPU support
 - Expanded storage metrics
 - On Demand integration
 - ColdFront integration
- **Application Kernel Development**
 - Support for cloud environments
 - Support for workflows
 - Develop Network usage Application Kernel



ACCESS Auditing

- ACCESS MMS will continue carrying out workload analyses on capability and capacity class systems as directed by NSF
- Similar to analyses carried out by XMS on Blue Waters and NSF Innovative Resources
 - Blue Waters Final Report: <https://arxiv.org/abs/1703.00924>
 - NSF Innovative Resources Final Report: <http://arxiv.org/abs/1801.04306>



Service Model – Data Service

- **Embrace the FAIR principles for scientific data**
 - **Findable**
 - The ACCESS XDMoD data warehouse will have a searchable metadata index that is both human and machine readable, publishing data and service assets
 - **Accessible**
 - Data warehouse assets will be available through standard REST calls. Metadata will be publicly available (Findable)
 - **Interoperable**
 - Data warehouse exports will be made available in commonly used machine readable formats including JSON and CSV
 - **Reusable**
 - MMS encourage reuse of XDMoD's data assets throughout the research community and will continue to do so



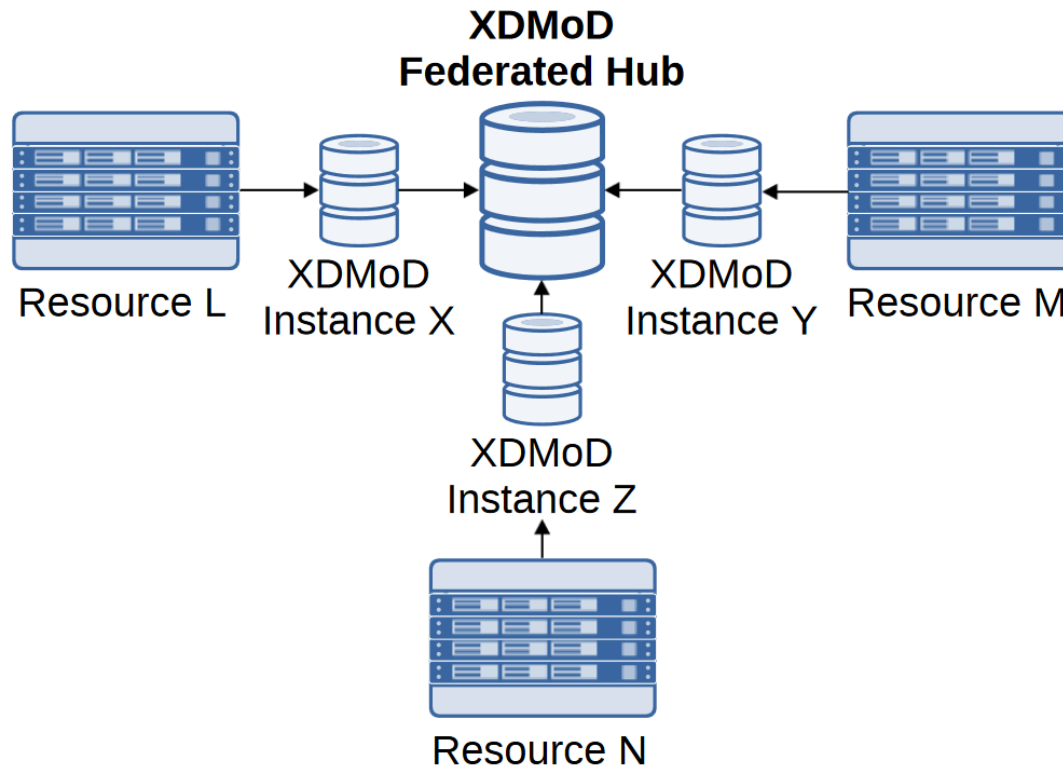
Service Model - ACCESS Tracks

- **Track 1 Allocations Service**
 - Historical CI usage for individual users/projects and overall CI resource usage
- **Track 2 End User Support Service**
 - Provide detailed information about end users historical jobs, workflow and network usage to help support and respond to customers' queries.
- **Track 3 Operations Service**
 - Provide information on ongoing ACCESS operations including QoS metrics
- **Track 5 Technology Translation**
 - Work with Track 5 and ACCESS ACO to determine and implement the proper reporting metrics
- **ACCESS ACO**
 - Provide information to support its management, oversight and coordination of the ACCESS awardees

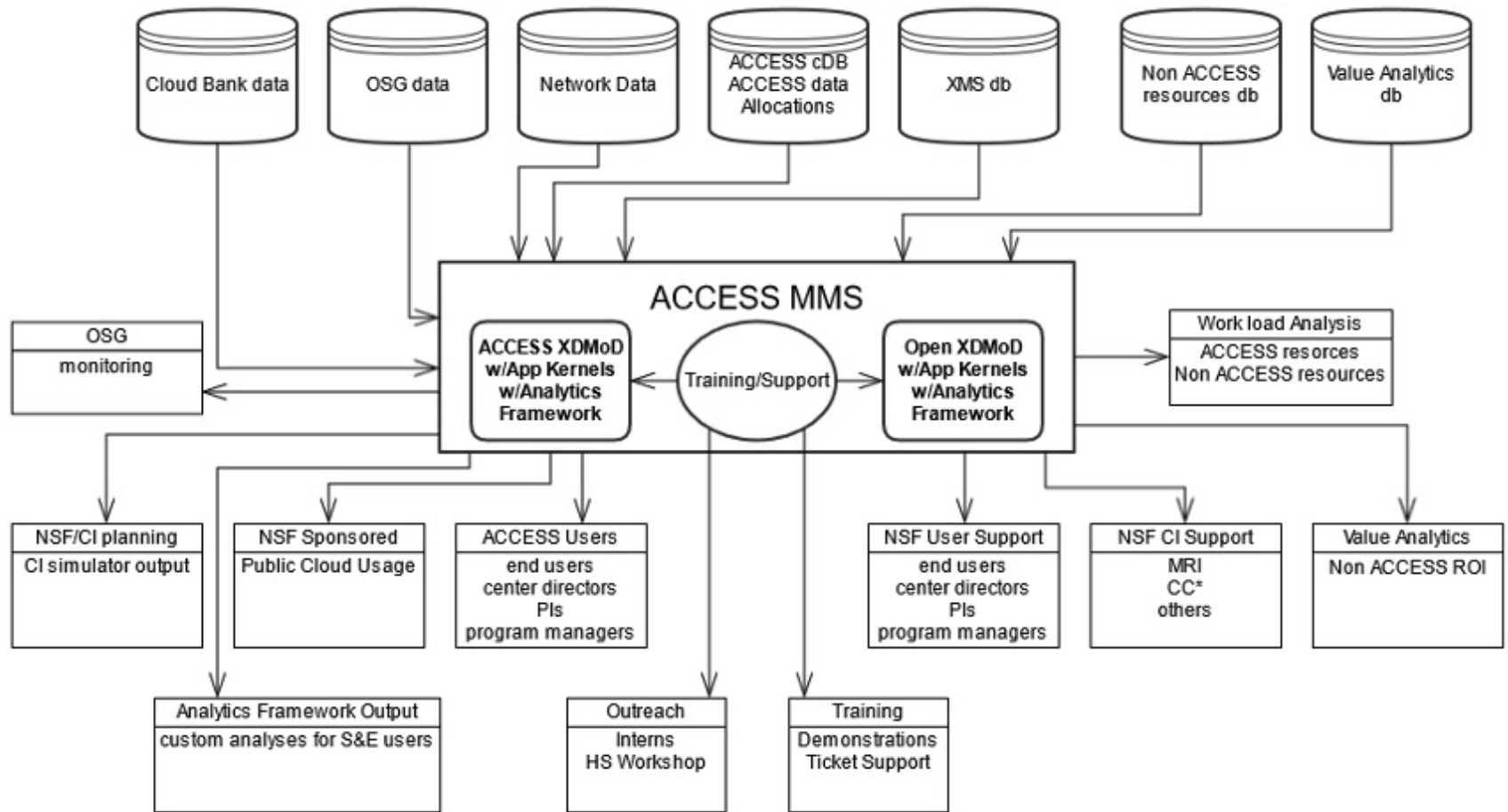


Federated XDMoD

- Federated XDMoD allows integration of multiple Open XDMoD instances into a single monitoring and reporting entity
- Can monitor each instance separately and/or look at the federation totals



ACCESS MMS Service Model Schematic



Discussion

