The Landscape of Academic Research Computing

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Chief Operations Officer – Software Assurance Marketplace
Manager High Throughput Computing

Let's jump right in…

$$
\begin{aligned}
E_n^{(1)} &= V_{nn} \\
E_n^{(2)} &= \frac{|V_{nk_2}|^2}{E_{nk_2}} \\
E_n^{(3)} &= \frac{V_{nk_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}} - V_{nn}\frac{|V_{nk_3}|^2}{E_{nk_3}^2} \\
E_n^{(4)} &= \frac{V_{nk_4}V_{k_4k_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}E_{nk_4}} - \frac{|V_{nk_4}|^2}{E_{nk_4}^2}\frac{|V_{nk_2}|^2}{E_{nk_2}} - V_{nn}\frac{V_{nk_4}V_{k_4k_3}V_{k_3n}}{E_{nk_3}^2E_{nk_4}} - V_{nn}\frac{V_{nk_4}V_{k_4k_2}V_{k_2n}}{E_{nk_2}E_{nk_4}^2} + V_{nn}^2\frac{|V_{nk_4}|^2}{E_{nk_4}^3} \\
&= \frac{V_{nk_4}V_{k_4k_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}E_{nk_4}} - E_n^{(2)}\frac{|V_{nk_4}|^2}{E_{nk_4}^2} - 2V_{nn}\frac{V_{nk_4}V_{k_4k_3}V_{k_3n}}{E_{nk_3}^2E_{nk_4}} + V_{nn}^2\frac{|V_{nk_4}|^2}{E_{nk_4}^3} \\
E_n^{(5)} &= \frac{V_{nk_5}V_{k_5k_4}V_{k_4k_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}E_{nk_4}E_{nk_5}} - \frac{V_{nk_5}V_{k_5k_4}V_{k_4n}}{E_{nk_4}^2E_{nk_5}}\frac{|V_{nk_2}|^2}{E_{nk_2}} - \frac{V_{nk_5}V_{k_5k_2}V_{k_2n}}{E_{nk_2}E_{nk_5}^2}\frac{|V_{nk_2}|^2}{E_{nk_2}} - \frac{|V_{nk_5}|^2}{E_{nk_5}^2}\frac{V_{nk_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}} \\
&\quad - V_{nn}\frac{V_{nk_5}V_{k_5k_4}V_{k_4k_3}V_{k_3n}}{E_{nk_3}^2E_{nk_4}E_{nk_5}} - V_{nn}\frac{V_{nk_5}V_{k_5k_4}V_{k_4k_2}V_{k_2n}}{E_{nk_2}E_{nk_4}^2E_{nk_5}} - V_{nn}\frac{V_{nk_5}V_{k_5k_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}E_{nk_5}^2} + V_{nn}\frac{|V_{nk_5}|^2}{E_{nk_5}^2}\frac{|V_{nk_3}|^2}{E_{nk_3}^2} + 2V_{nn}\frac{|V_{nk_5}|^2}{E_{nk_5}^3}\frac{|V_{nk_2}|^2}{E_{nk_2}} \\
&\quad + V_{nn}^2\frac{V_{nk_5}V_{k_5k_4}V_{k_4n}}{E_{nk_4}^3E_{nk_5}} + V_{nn}^2\frac{V_{nk_5}V_{k_5k_3}V_{k_3n}}{E_{nk_3}^2E_{nk_5}^2} + V_{nn}^2\frac{V_{nk_5}V_{k_5k_2}V_{k_2n}}{E_{nk_2}E_{nk_5}^3} - V_{nn}^3\frac{|V_{nk_5}|^2}{E_{nk_5}^4} \\
&= \frac{V_{nk_5}V_{k_5k_4}V_{k_4k_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}E_{nk_4}E_{nk_5}} - 2E_n^{(2)}\frac{V_{nk_5}V_{k_5k_4}V_{k_4n}}{E_{nk_4}^2E_{nk_5}} - \frac{|V_{nk_5}|^2}{E_{nk_5}^2}\frac{V_{nk_3}V_{k_3k_2}V_{k_2n}}{E_{nk_2}E_{nk_3}} \\
&\quad - 2V_{nn}\left(\frac{V_{nk_5}V_{k_5k_4}V_{k_4k_3}V_{k_3n}}{E_{nk_3}^2E_{nk_4}E_{nk_5}} - \frac{V_{nk_5}V_{k_5k_4}V_{k_4k_2}V_{k_2n}}{E_{nk_2}E_{nk_4}^2E_{nk_5}} + \frac{|V_{nk_5}|^2}{E_{nk_5}^2}\frac{|V_{nk_3}|^2}{E_{nk_3}^2} + 2E_n^{(2)}\frac{|V_{nk_5}|^2}{E_{nk_5}^3}\right) \\
&\quad + V_{nn}^2\left(2\frac{V_{nk_5}V_{k_5k_4}V_{k_4n}}{E_{nk_4}^3E_{nk_5}} + \frac{V_{nk_5}V_{k_5k_3}V_{k_3n}}{E_{nk_3}^2E_{nk_5}^2}\right) - V_{nn}^3\frac{|V_{nk_5}|^2}{E_{nk_5}^4}
\end{aligned}
$$

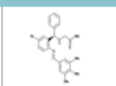
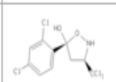
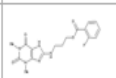
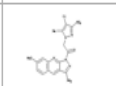
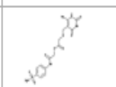
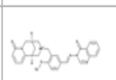
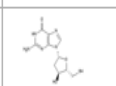
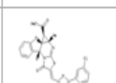
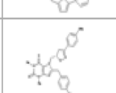
Who Am I?

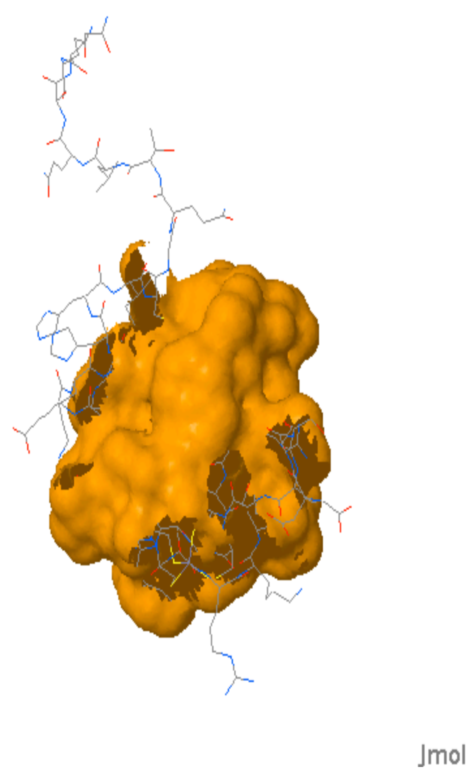
- Chief Operations Officer of the Open Science Grid and Software Assurance Marketplace – 10+ years
- Manager High Throughput Computing Indiana University (IU)
- IU Institutional OSG PI
- Co-PI Science Node – (Formally - International Science Grid This Week)
- External Advisor to European Grid Infrastructure
- Member of the Organizational Advisory Board for RDA

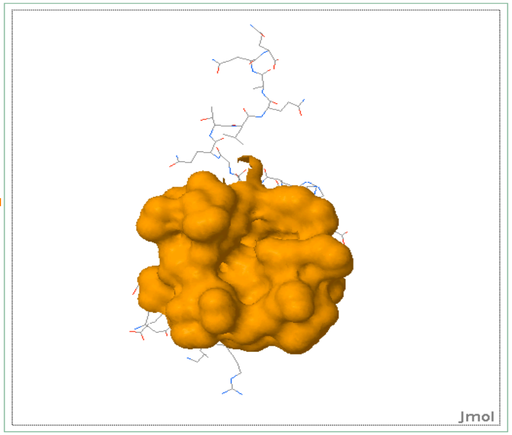
Protein Docking Project at the IU School of Medicine

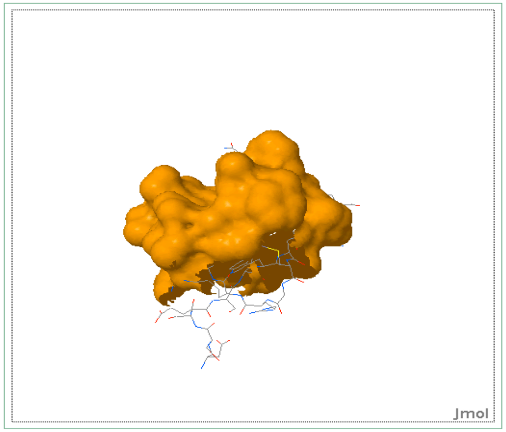
- SPLINTER - Structural Protein-Ligand Interactome
- Used autodock-vina – "…open-source program for drug discovery, molecular docking and virtual screening…"
- Frist run in 2013 - docked ~3900 Proteins with 5000 Ligands for a total of ~19M docked pairs.
- Submitted via command line to Condor using Pegasus on the OSG-XSEDE submission node
- Infrastructure is set and new runs can be easily started

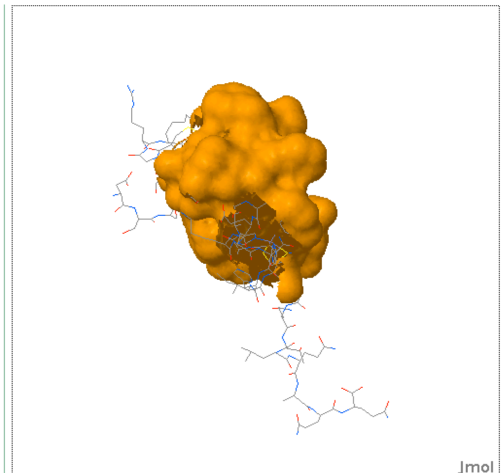
•Various rotations of Protein CBFA2T1 (Cyclin-D-related protein) (Eight twenty one protein) (Protein ETO) (Protein MTG8) (Zinc finger MYND domain-containing protein 2)

Target	Ligand Image	Rank
ZINC27470710 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		1
ZINC01228697 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		2
ZINC04741379 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		3
ZINC09611213 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		4
ZINC02810311 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		5
ZINC02945941 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		6
ZINC00404256 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		7
ZINC20038318 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		8
ZINC04039256 VIEW POSE MOL2 ORDER INFO OTHER TARGETS		9





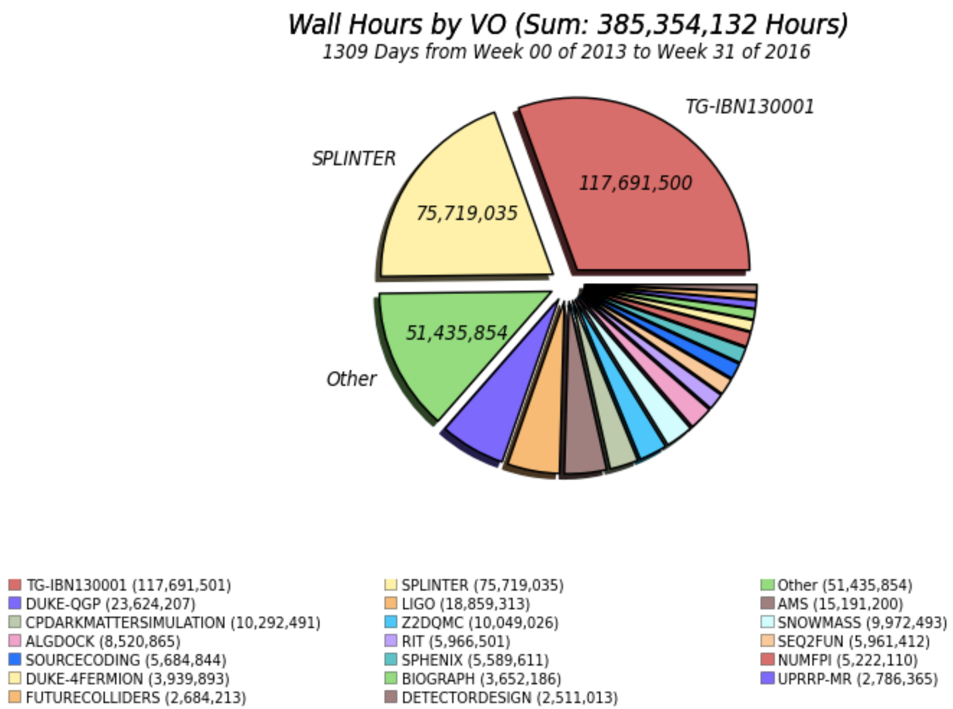




Open Science Grid

Some Numbers

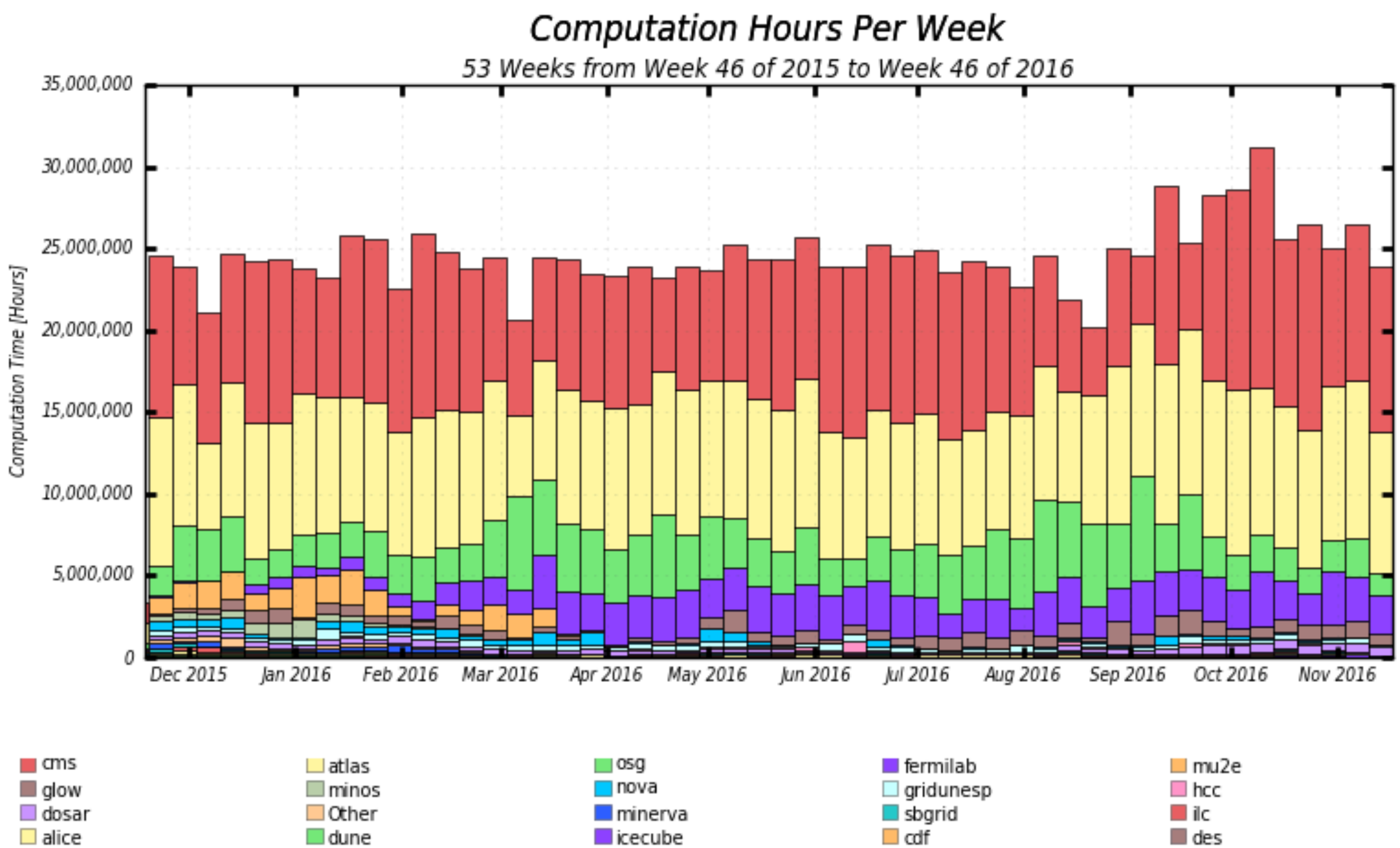
RESEARCH DATA ALLIANCE U.S.



- Amazon EC2 Computing $0.073/hour
- $5.5M Compute Only
- Data Transfer and Storage Not Included

At what scale?

Job Activity



Most important!

- Please ask questions!

  …during the lectures

  …during the exercises

  …after class

  …via email after we depart (rquick@iu.edu)

- If I don't know, I'll find the right person to answer your question.

Goals for this session

- Define Local, Clustered, High Throughput Computing (HTC), High Performance Computing (HPC), and Cloud Computing (XaaS)

- Shared, Allocated, and Purchased

The setup: You have a problem

- Your research computing is complex!
  - Monte carlo, image analysis, genetic algorithm, simulation, text mining…
- It will take a year to get the results on your laptop, but the conference is in a week.
- What do you do?

Option 1: Wait a year

Option 2: Local Clustered Computing

- Easy access to additional nodes
- Local support for porting to environment (maybe)
- Often a single type of resource
- Often running at capacity
- At IU these machines are called: Big Red 2, Karst, and Mason

Option 3: Use a “supercomputer” aka High Performance Computing(HPC)

- “Clearly, I need the best, fastest computer to help me out”
- Maybe you do…
  - Do you have a highly parallel program?
    - i.e. individual modules must communicate
  - Do you require the fastest network/disk/memory?
- Are you willing to:
  - Port your code to a special environment?
  - Request and wait for an allocation?

Option 4: Use lots of commodity computers

- Instead of the fastest computer, lots of individual computers
- May not be fastest network/disk/memory, but you have a lot of them
- Job can be broken down into separate, independent pieces
  - If I give you more computers, you run more jobs
  - You care more about total quantity of results than instantaneous speed of computation
- This is **high-throughput computing (HTC)**

Option 5: Buy (or Borrow) some computing from a Cloud Provider

- Unlimited resources (if you can afford them)
- Full administrative access to OS of the resources you ‘buy’
- Specialized VM images reducing effort in porting
- XaaS Business Model

These are All Valid Options

- Remember the problem you have one month to publish results for your conference
  - Option 1: You will miss your deadline
  - Option 2: You might miss your deadline – But if your lucky you'll make it (or if you know the admin)
  - Option 3: If you have parallelized code and can get an allocation you have a good chance
  - Option 4: If you can serialize your workflow you have a good chance
  - Option 5: You can meet your deadline for a price. Though some efforts are underway to enable academic clouds.

Computing Infrastructures

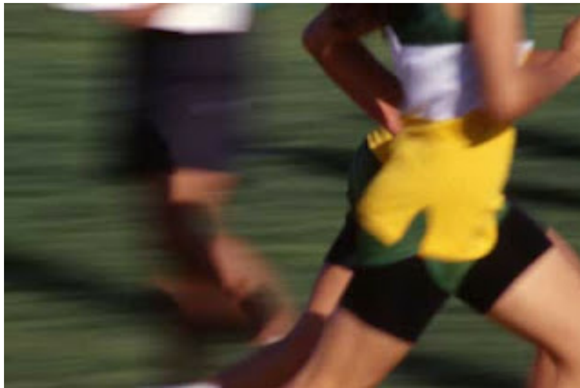
- Local Laptop/Desktop – Short jobs with small data
- Local Cluster – Larger jobs and larger data but subject to availability
- HPC – Prime performance with parallelized code
- HTC – Sustained computing over a long period for serialized
- Cloud – Need deeper permission on an OS and have deeper pockets

Why do I focus on high-throughput computing? (HTC)

- An approach to distributed computing that focuses on long-term throughput, not instantaneous computing power
  - We don't care about operations per second
  - We care about operations per year
- Implications:
  - Focus on reliability
  - Use all available resources
    - Any Linux based machine can participate

Think about a race

- Assume you can run a four minute mile
- Does that mean you can run a 104 minute marathon?
- The challenges in sustained computation are different than achieving peak in computation speed



Openness

- In an era of Open Data and Open Science shouldn't the computing also be as open as possible?
- I think HTC has the best opportunity to contribute to Open Science.
- Anyone can use or contribute resources for research purposes.

Why is HTC hard?

- The HTC system has to keep track of:
  - Individual tasks (a.k.a. jobs) & their inputs
  - Computers that are available
- The system has to recover from failures
  - There will be failures! Distributed computers means more chances for failures.
- You have to share computers
  - Sharing can be within an organization, or between orgs
  - So you have to worry about security
  - And you have to worry about policies on how you share
- If you use a lot of computers, you have to handle variety:
  - Different kinds of computers (arch, OS, speed, etc..)
  - Different kinds of storage (access methodology, size, speed, etc…)
  - Different networks interacting (network problems are hard to debug!)

Open Science Grid

Jetstream

A Introduction to Jetstream

Jetstream: A national research and education cloud
The ECSS/Staff Edition

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With Modifications for the CODATA/RDA Summer School in Data Science by Rob Quick
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Award #ACI-1445604

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What is cloud computing?

- Wikipedia says *“Cloud computing is the use of computing resources (hardware and software) that are delivered as a service over a network (typically the Internet). The name comes from the common use of a cloud-shaped symbol as an abstraction for the complex infrastructure it contains in system diagrams. Cloud computing entrusts remote services with a user's data, software and computation.”*

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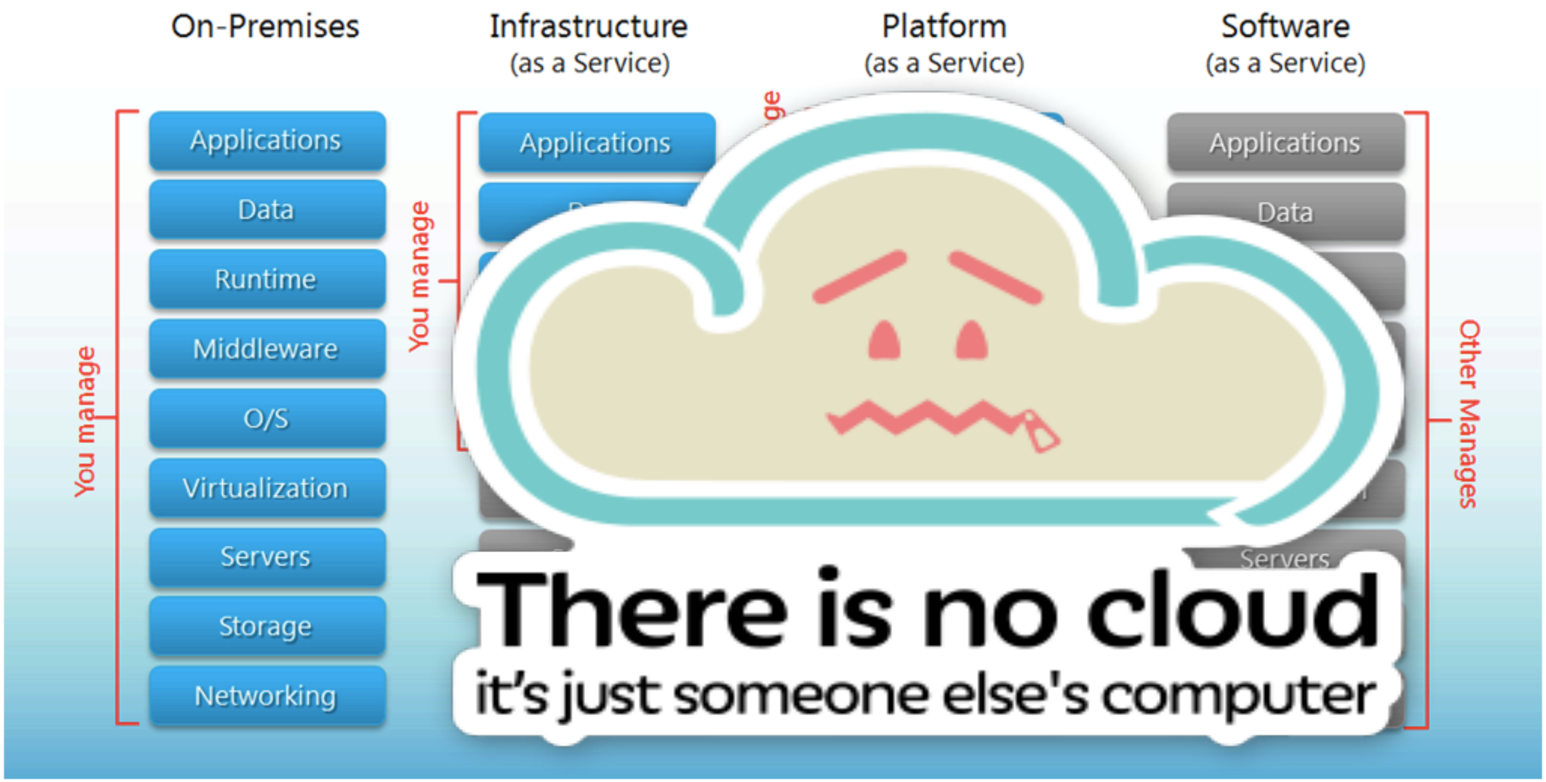

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What is Jetstream?

- A resource to *expand the community of users* who benefit from investments in shared cyberinfrastructure
- *Production cloud system* supporting all domains of science and engineering research
- Provide on-demand *interactive* computing and analysis
- Enable *configurable* environments and architectures
- Support computational *reproducibility and sharing*
- Democratizes access to *cloud-native* technology and software
- Focuses on *ease of use*, but also on *maintaining flexibility*

NSF
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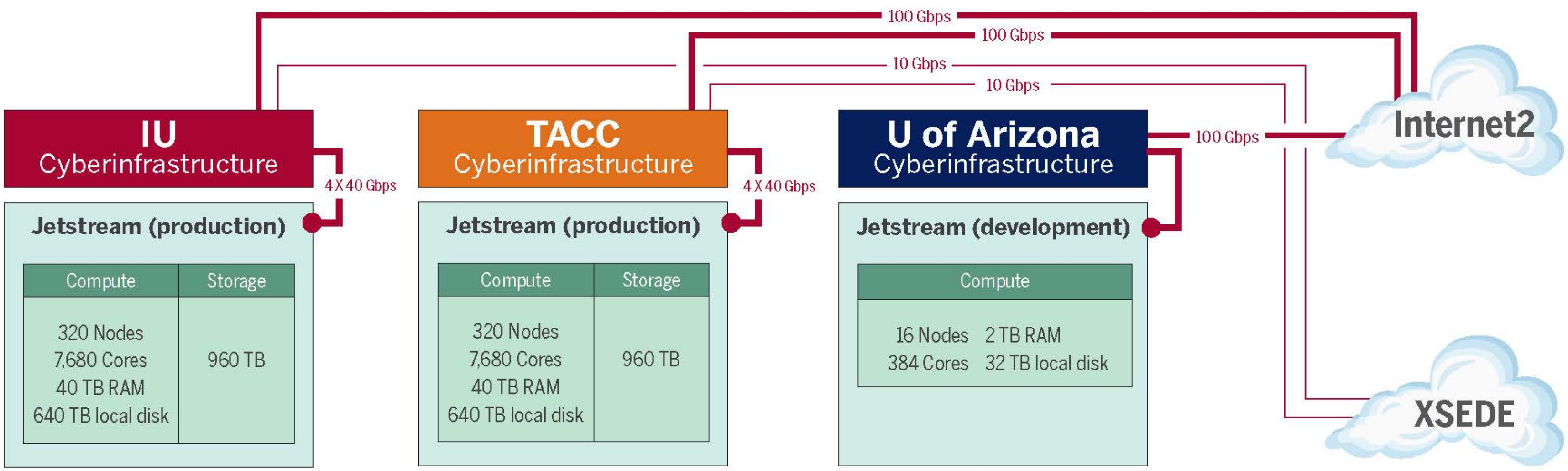
Jetstream System Overview



http://jetstream-cloud.org/

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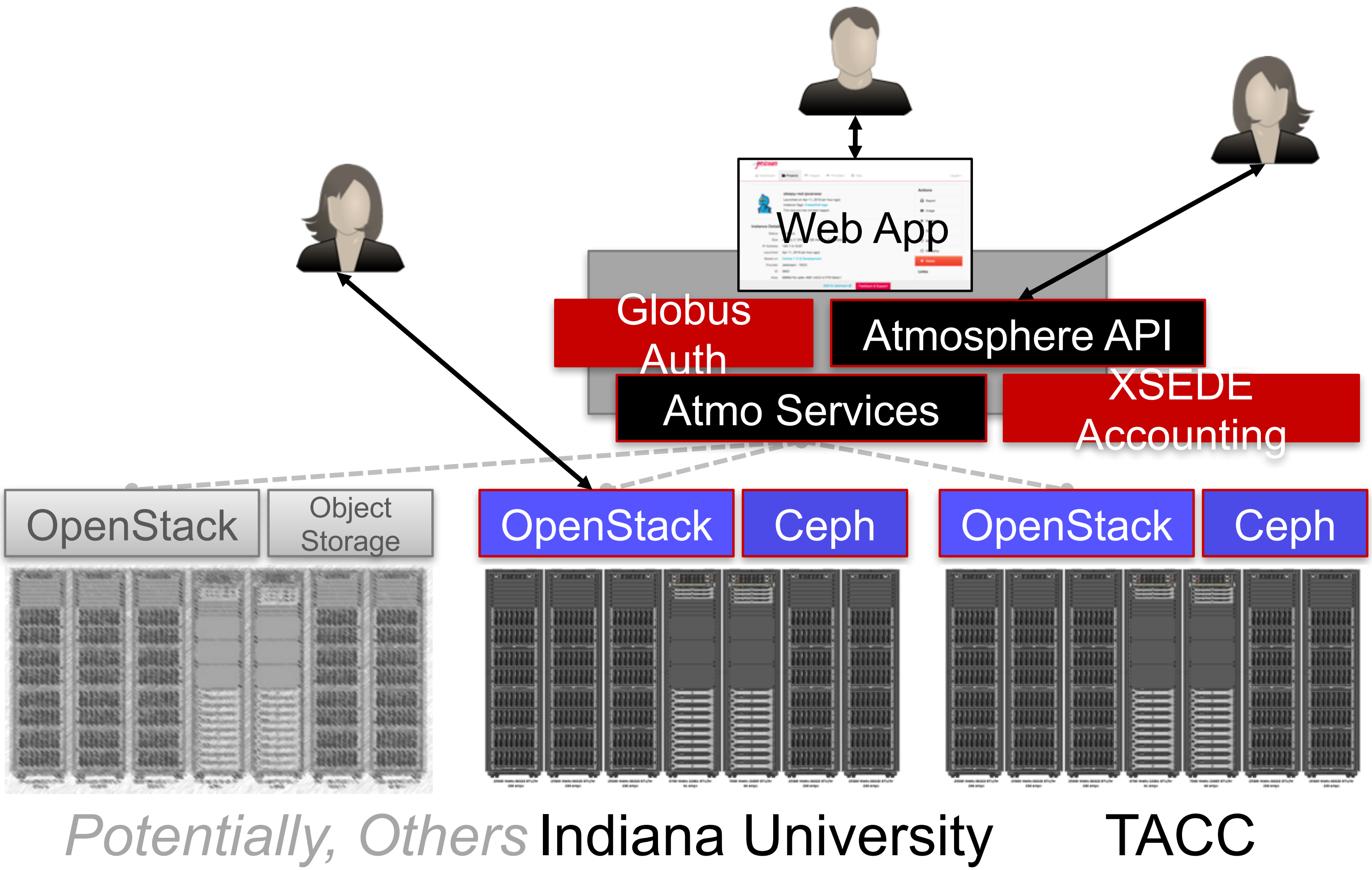
Platform Overview



Levels of access

Two levels of access

- Interactive user access via web interface and vnc/ssh
- Persistent access for Science Gateways and other “always on” services or services launched programmatically on demand; e.g. elastic compute techniques

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Hardware and Instance "Flavors"

VM Host Configuration

- Dual Intel E-2680v3 "Haswell"
- 24 physical cores/node @ 2.5 GHz (Hyperthreading on)
- 128 GB RAM
- Dual 1 TB local disks
- 10GB dual uplink NIC
- Running KVM Hypervisor

Flavor	vCPUs	RAM	Storage	Per Node
m.tiny	1	2	8	46
m.small	2	4	20	23
m.medium	6	16	60	7
m.large	10	30	120	4
m.xlarge	24	60	240	2
m.xxlarge	44	120	480	1

- Short-term storage comes as part of launched instance
- Long-term storage is XSEDE-allocated
- Implemented on backend as OpenStack Volumes
- Each user gets 10 volumes up to 500GB total storage
- Piloting object storage as well after recent update

Open Science Grid

Where can I learn more?

- Production:
  - Wiki: http://wiki.jetstream-cloud.org
  - User guides: https://portal.xsede.org/user-guides
  - XSEDE KB: https://portal.xsede.org/knowledge-base
  - Campus Champions: https://www.xsede.org/campus-champion

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Open Science Grid

Project website: http://jetstream-cloud.org/
Project email: help@jetstream-cloud.org Direct email: jeremy@iu.edu

License Terms

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Accessing Jetstream

- First time, you should log into Atmosphere and accept the terms from Globus and XSEDE
- See the GUI – know what most end users might see
- The other reason(s)? It's good to know the GUI so you can disregard it? ☺
- GUI vs API in terms of use

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Data and the ins and outs

- Moving data in and out…well, that's up to you
  - Globus on Atmosphere
  - Globus on API VMs
- Backups
  - Punchcards
  - Jetstream proper
  - VMs
  - Snapshots
- Let's talk about storage in general...

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Image preservation and publication

- Part of the "what makes Jetstream unique" design is the plan for long term image storage
- When you're ready:

  http://www.jetstream-cloud.org/request-doi-test.php
- The result (a sample):

  http://doi.org/10.5967/P9H59R (Old style IUSW)

  https://scholarworks.iu.edu/iuswrdemo/handle/123456789/20894

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Thank you for your attention

Please feel free to contact me any time and ask questions. If you'd like access to HTC Resources (OSG) or to know more about JetStream. (rquick@iu.edu)

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Questions?

- Questions? Comments?
  - Feel free to ask me questions now or later:
    Rob Quick rquick@iu.edu

Exercises start here:

https://twiki.grid.iu.edu/bin/view/Sandbox/JetStreamTutorial

Slides are also available from this URL.