



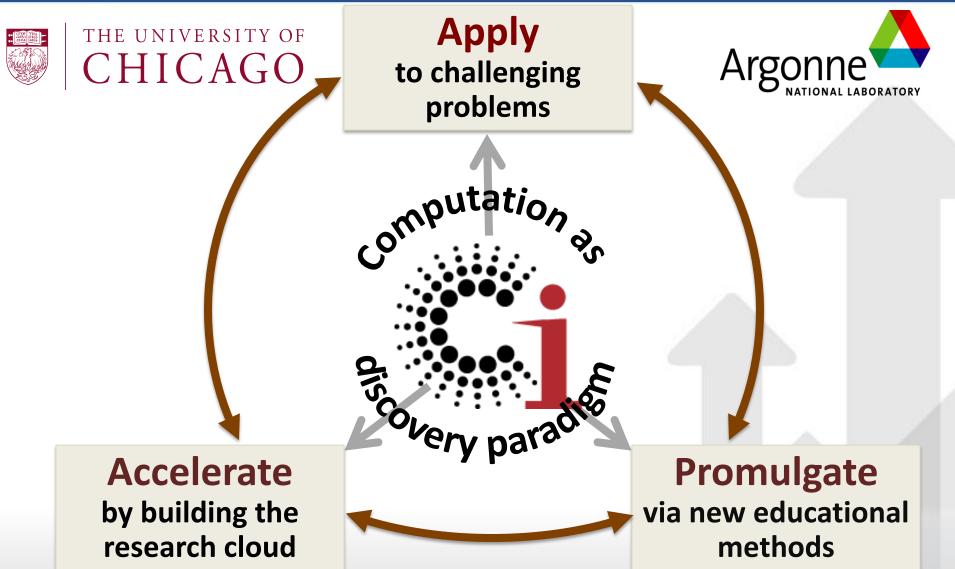
Cloud-based services for (reproducible) science

Ian Foster

Computation Institute
University of Chicago and Argonne National Laboratory



Computation Institute (CI)



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Software-as-a-Service (SaaS)

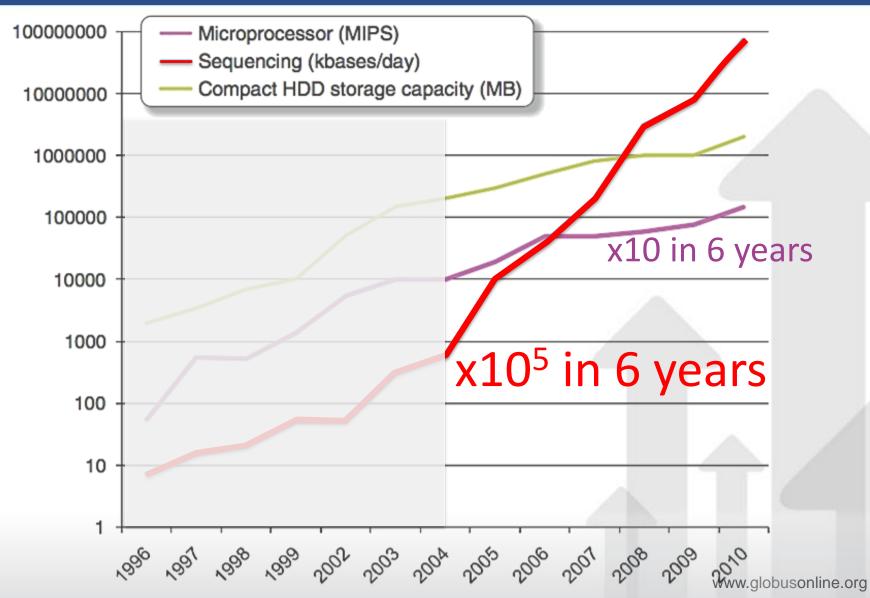
Platform-as-a-Service (PaaS)

Infrastructure-as-a-Service (IaaS)



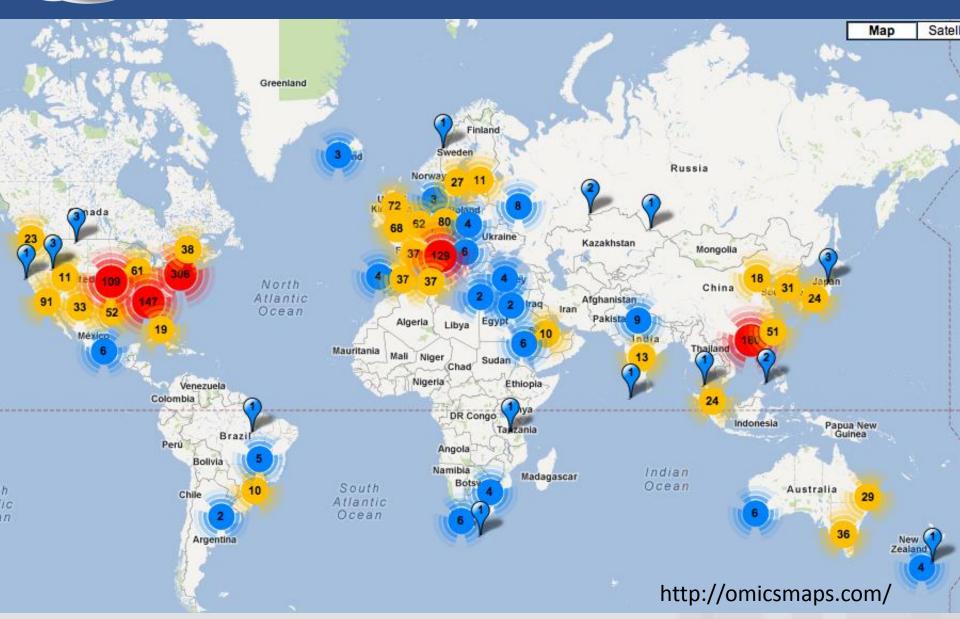


The data deluge in biology





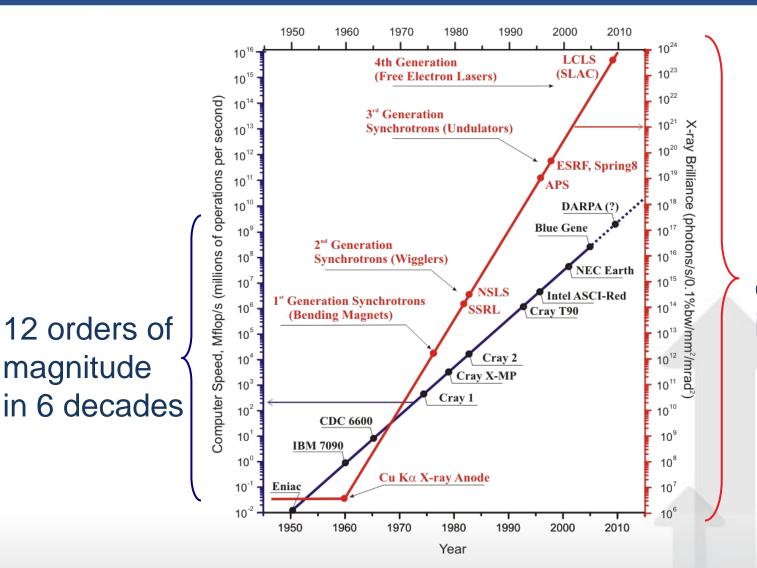
Number of sequencing machines





magnitude

Moore's Law for X-ray sources



18 orders of magnitude in 5 decades!

Credit: Linda Young

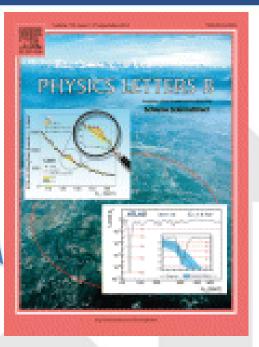
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Big science has been successful



15 PB/year 173 TB/day 500 MB/sec Globus GridFTP
300K files/day
0.3 PB/day
... just for LHC



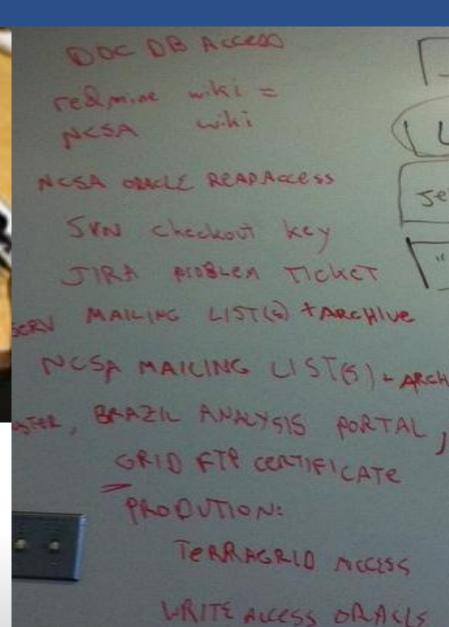




But small and medium science is suffering

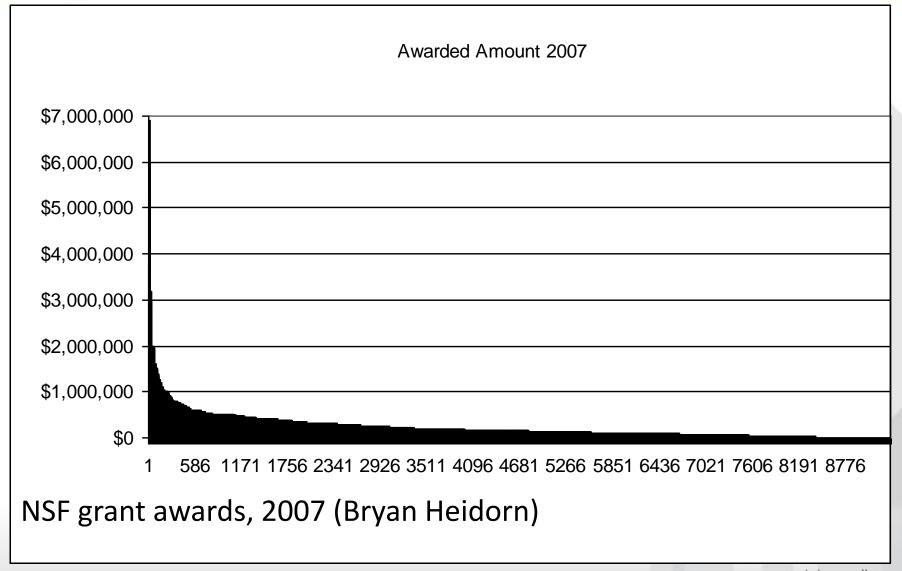


- Data deluge
- Ad-hoc solutions
- Inadequate software, hardware & IT staff





Dark data in the long tail of science





A crisis that demands new approaches

- We have **exceptional infrastructure for the 1%** (e.g., supercomputers, Large Hadron Collider, ...)
- But **not for the 99%** (e.g., the vast majority of the 1.8M publicly funded researchers in the EU)

We need new approaches to providing research cyberinfrastructure, that:

- Provide advanced functionality
- Reduce barriers to entry
- Are cheaper
- Are sustainable



Run a research project from a coffee shop?

STARBUC (S COFFE





Rethinking how we provide research IT

Accelerate discovery and innovation worldwide by providing research IT as a service

Leverage the cloud to

- provide millions of researchers with unprecedented access to powerful tools;
- enable a massive shortening of cycle times in time-consuming research processes; and
- reduce research IT costs dramatically via economies of scale



Time-consuming Tasks in Research

- Run experiments
- Collect data
- Manage data

- Communicate with colleagues
- Publish papers
- "Civilization advances by extending the number of important operations which we can perform without thinking of them"

—Alfred North Whitehead, 1911

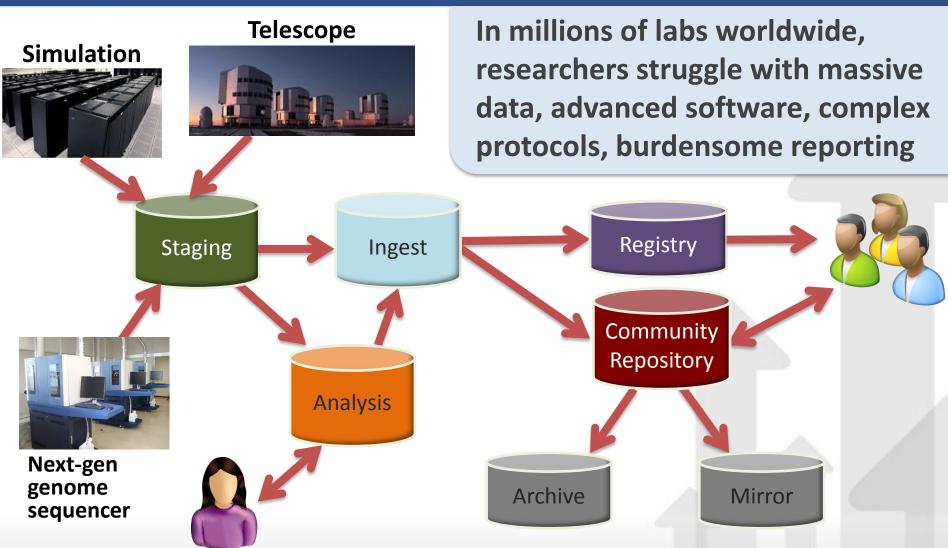
- Kun simulations
- Compare experiment with simulation
- Search the literature

- Order supplies
- Write proposals
- Write reports

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Addressing the big data challenge



Accelerate discovery and innovation by outsourcing difficult tasks



Grid meets Cloud

Millions of researchers worldwide need advanced IT to tackle important and urgent problems



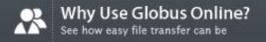


Reliable, high-performance, secure file transfer.

Move files fast. No IT required.













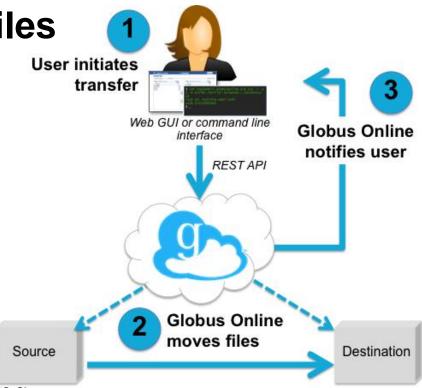
What is Globus Online?

Transfer and synchronize files

- Easy "fire-and-forget" transfers
- Automatic fault recovery
- High performance
- Across multiple security domains

Minimize IT costs

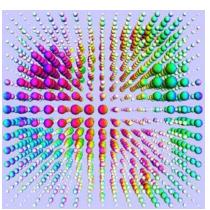
- Software as a Service (SaaS)
 - No client software installation
 - · New features automatically available
- Consolidated support & troubleshooting
- Simple endpoint installation with Globus Connect and GridFTP
- Recommended by XSEDE, Blue Water, NERSC, ALCF, ESnet, many Universities





Case Study: Lattice QCD

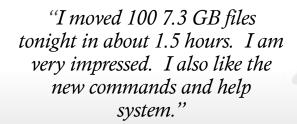




"Globus Online frees up my time to do more creative work than typing scp commands or devising scripts to initiate and monitor progress to move many files."

- Fast: Reduced transfer times
- Easy: Fire-and-forget transfers
 - Automated retry
 - No file pre-staging
 - No complex infrastructure
 - Convenient CLI and GUI interfaces.

Indiana University researcher moved ~6 TB from Tennessee to Texas in 2 days







Case Study: Enabling Users @ NERSC

Challenge

- "We need to provide web-based ways to accomplish computing tasks – it's what our scientists expect. And it will make them more productive."

Solution

- Globus Online endpoints maintained by NERSC
- Globus = recommended transfer method

Benefits for NERSC users

- Drag and drop archiving
- Easy to use
- Users can focus on their research (not on IT)

Benefits for NERSC

- Operations and support outsourced to Globus
- Fast and easy to make endpoints available
- Automated authentication
- Reliable performance and support



"Fantastic! I have already started using Globus Connect to transfer data, and it only took me 5 minutes to set up. Thank you!" – NERSC user



Hopper, Franklin and HPSS are among the NERSC resources leveraged by Globus Online.























SIGN IN SIGN UP

Reliable, high-performance, secure file transfer by Globus Online.

Blue Waters has partnered with the Globus Online file transfer service.

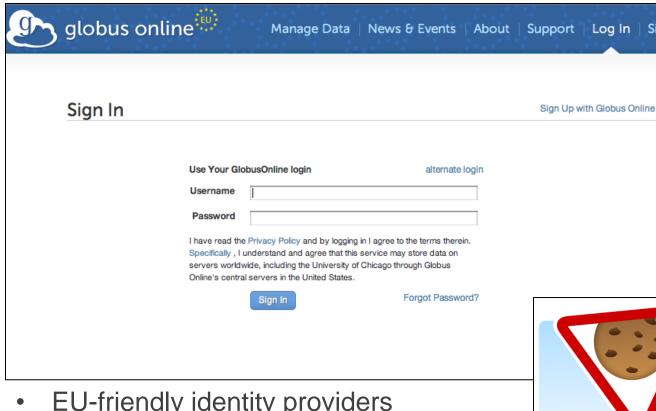
You may access this service by entering your Blue Waters username and password.

NOTE - If you are accessing this file transfer service for the first time, you will be asked to link your Blue Waters account to a Globus Online account (if you don't have a Globus Online account you'll be able to create one).





globusonline.eu



Partners





Enter Site

- EU-friendly identity providers
- EU relevant endpoints
- Integrated support with EGI & IGE
- **EU Cookie Law compliant**
- Consent to store log data in US



Platform-as-a-Service (PaaS)

Infrastructure-as-a-Service (IaaS)

Deliver advanced functionality that:

- Requires no user software installation or operation
 - Minimal IT proficiency required
- Can be cheaply and incrementally adopted
 - Usage-based subscription pricing; no big up-front costs
- Consolidates troubleshooting and support
 - An expert group can proactively detect and correct problems
- Utilizes an efficient software delivery lifecycle
 - Updates developed, tested and deployed quickly

Dominates commercial & consumer markets

– What about the research market?



Software as a Service (SaaS) vs. traditional software delivery

- SaaS changes assumptions and approach throughout the software lifecycle
 - Architecture and design
 - Designed for specific environment (e.g., AWS)
 - Software development
 - No porting or cross platform testing. Focus on functionality.
 - Operations
 - Continuous update cycle. Nobody else will operate.
 - Focus on availability, automation, monitoring
 - Support
 - Tightly integrated with operations
- We are delivering a service, not software



Potential economies of scale

Small laboratories

- PI, postdoc, technician, grad students
- Estimate 10,000 across US research community
- Average ill-spent/unmet need of 0.5 FTE/lab?

+ Medium-scale projects

- Multiple Pls, a few software engineers
- Estimate 1,000 across US research community
- Average ill-spent/unmet need of 3 FTE/project?
- = Total 8,000 FTE: at ~\$100K/FTE => \$800M/yr (If we could even find 8,000 skilled people)

Plus computers, storage, opportunity costs, ...



SaaS and reproducible publications

- Hosted services can contribute to relieving author burden
- Store data, code, and workflows
- Maintain bindings among data, code, executions, workflows, provenance
- Etc.

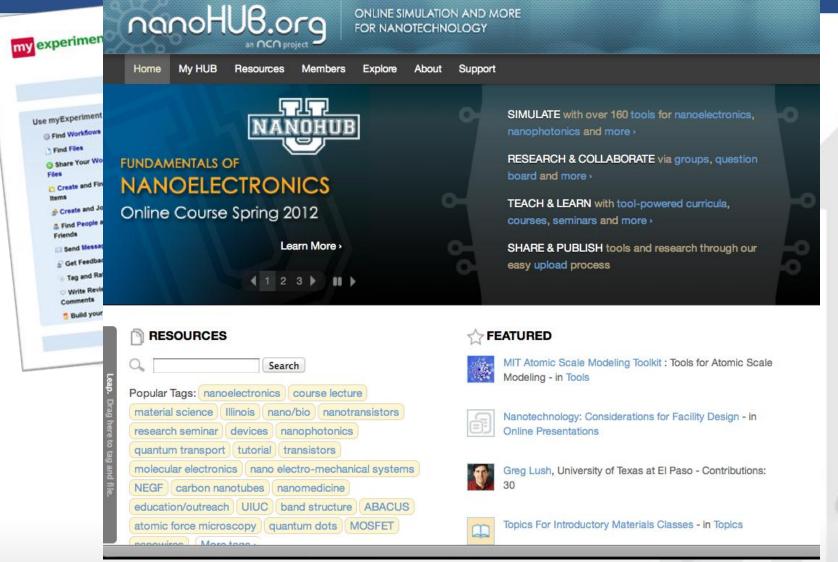


Other innovative science SaaS projects





Other innovative science SaaS projects

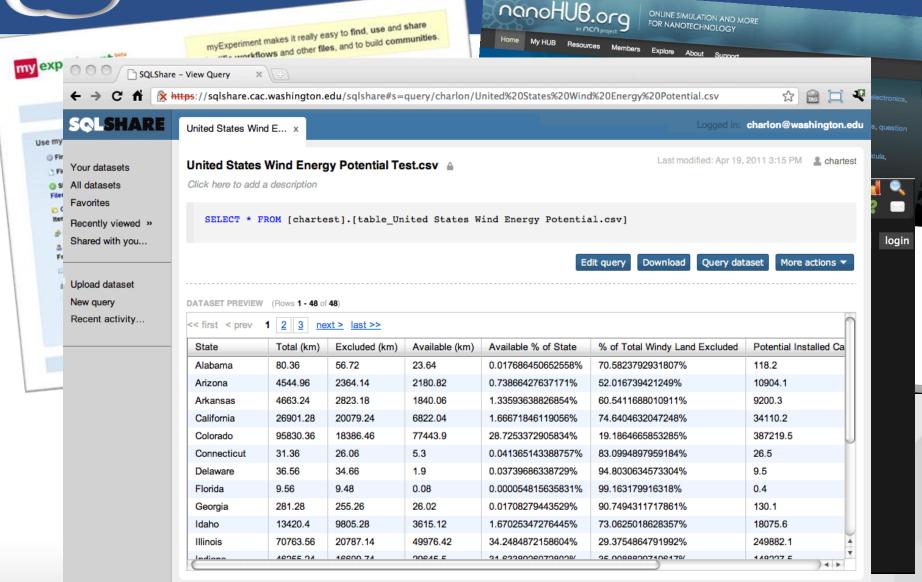


Other innovative science SaaS projects myExperiment makes it really easy to find, use and share scientific workflows and other files, and to build communities. my experiment --login metagenomics analysis server Browse Metagenomes search for metagenomes Register **Contact** Help Upload **About** MG-RAST (the Metagenomics RAST) server is an automated analysis platform for metagenomes providing quantitative insights into microbial populations based on sequence data. The server provides web based upload, quality control, automated # of metagenomes 35.586 annotation and analysis for samples up to 10GBp. Comparison # base pairs 9.24 Tbp between large numbers of samples is enabled via pre-computed abundance profiles. MG-RAST was launched in 2007 and has # of sequences 85.21 billion over 5000 registered users and 35,586 data sets. The current # of public metagenomes 7,167 server version is 3.1.2.

MG-RAST Version 3.1.2 released

Updates

Other innovative science SaaS projects



Other innovative science SaaS projects mvExperiment makes it really easy to find, use and share FOR NANOTECHNOLOGY tiles, and to build communities. iPlant Collaborative Web Port × **→8** ☆ ① 🔀 www.iplantcollaborative.org Contact Us Login or Register Feedback iPlant Collaborative™ Empowering A New Plant Biology Challenge iPlant develops a vision for 000 ← → 0 ezneiza inalg login SQLS cyberinfrastructure Your datase All datasets Favorites Recently vi CHALLENGE DISCOVER CONNECT LEARN Shared with Upload data iPlant Genotype to Discovery **Upcoming Events** People at iPlant New query Recent act Phenotype (iPG2P) Environment Community driven science iPlant Tools and Services Workshop @ University of Missouri, Columbia Mapping the links Access iPlant tools (FULL WORKSHOP) between genotypes and through a single user-LOGIN September 24 2012 - September 25 2012 friendly interface phenotypes · iPlant Genomics in Education MORE... Barcoding Workshop @ SACNAS, Seattle iPlant Tree of Life October 10 2012 **DNA Subway** (iPToL) · iPlant Genomics in Education An educator-tailored Workshop @ Schoolcraft College -Understanding the interface for bringing

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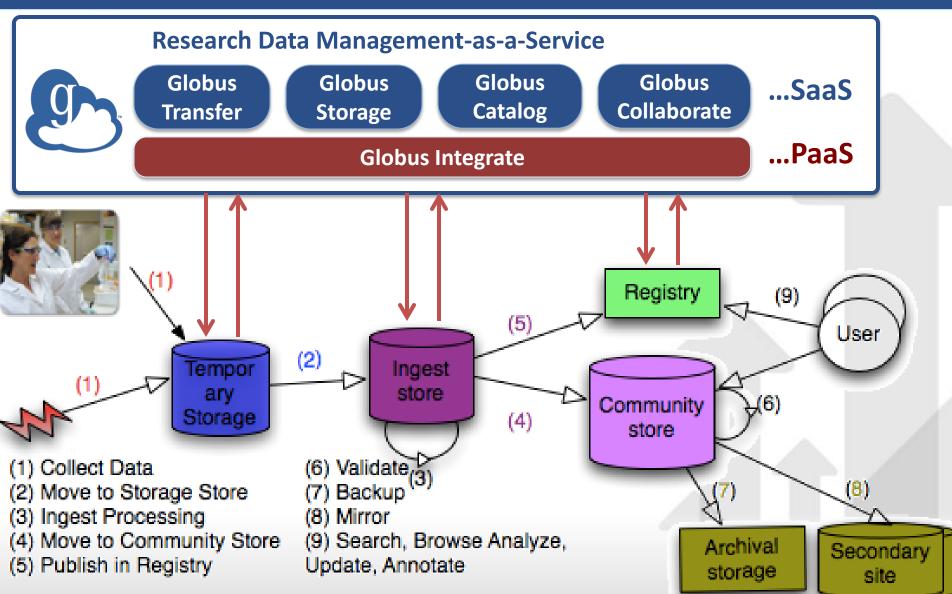
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Other innovative science SaaS projects nanoHUB.org ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY sy to find, use and share runmycode uild communities. Home My HUB Resources **→ 8** ☆ ① 🔀 Home First visit? Our offering Login or Register Feedback Submit your code The concept Use Search by themes Advanced search Search here ... As simple as 1,2,3 Help/FAQ 1. A researcher has an idea. Our partners Search 2. The researcher writes a paper The team 000 Contact us based on this idea. 3. Using RunMyCode, the researcher ← → C creates a companion website SQL associated with this paper. The companion website allows people to Your data implement the methodology presented All datas Favorit Recen Learn more >> Рарег About Concept Purpose iPlant Tree of Lite (iPToL) An educas. Understanding the interface for bringing Create your own companion website >> 13420.4 9805.28 3615.12 1.67025347276445% 73.06250100 Illinois 70763.56 20787.14 49976.42 29.3754864791992% ne.org



Towards "research IT as a service"





PaaS for Research

Software-as-a-Service (SaaS)

Platform-as-a-Service (PaaS)

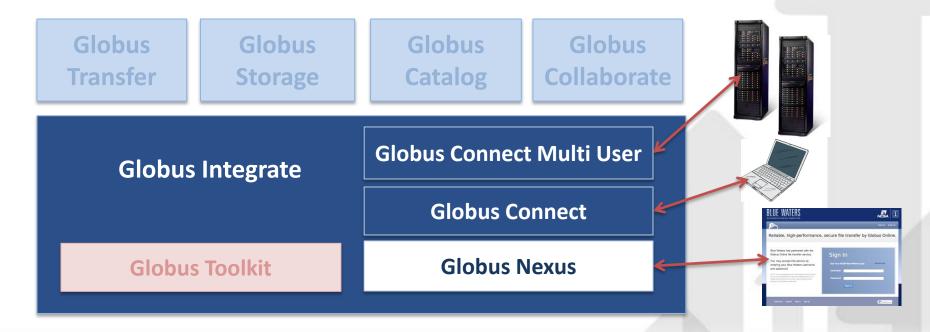
Infrastructure-as-a-Service (IaaS)

- No one SaaS provider can deliver it all
- Must create ecosystem that:
 - Allows any SaaS provider to easily participate
 - Dramatically reduces the cost of creating and operating services within the ecosystem
 - Provides seamless user experience across services
 - Agnostic to / works across any cloud laaS provider
- Ecosystem requires Platform as a Service
 - Target the unique needs of the research community



Globus Integrate: For when you want to...

- Integrate with the Globus research cloud ecosystem
- Write programs that leverage:
 - (federated) user identities, profiles, groups
 - data, compute and collaboration



... via REST APIs and command line programs



Dark Energy Survey – Leveraging transfer

Blanco 4m on Cerro Tololo

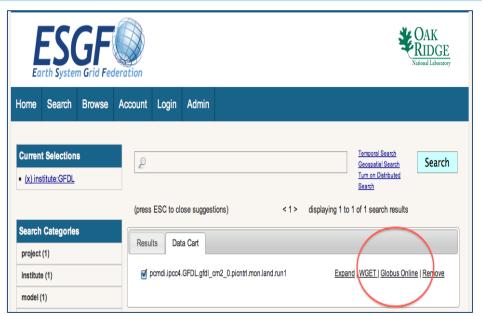
- Every night, they receive 100,000 files in Illinois
- They transmit files to
 Texas for analysis ...
 then move results back to
 Illinois ...
 and make them available to
 users
- Process must be reliable, routine, and efficient
- The cyberinfrastructure team is not large!



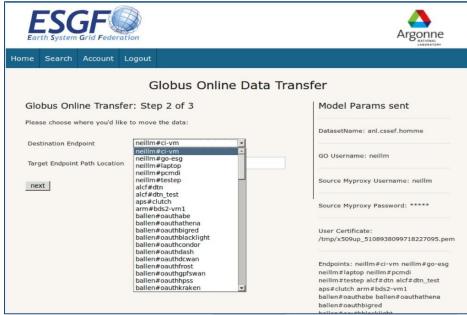
Image credit: Roger Smith/NOAO/AURA/NSF



Earth System Grid – Portal integration



- Outsource data transfer to Globus
 - Data download to user machine from search
 - Data transfer to another server by user
 - Replication of data between sites by administrator
- No ESGF client software needed







KBase – Leveraging the full platform

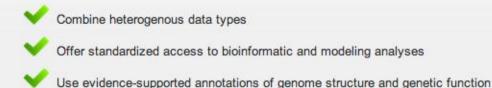


The new Systems Biology Knowledgebase (KBase) is a

collaborative effort designed to accelerate our understanding of microbes, microbial communities, and plants. It will be a community-driven, extensible and scalable open-source software framework and application system. KBase will offer free and open access to data, models and simulations, enabling scientists and researchers to build new knowledge and share their findings.



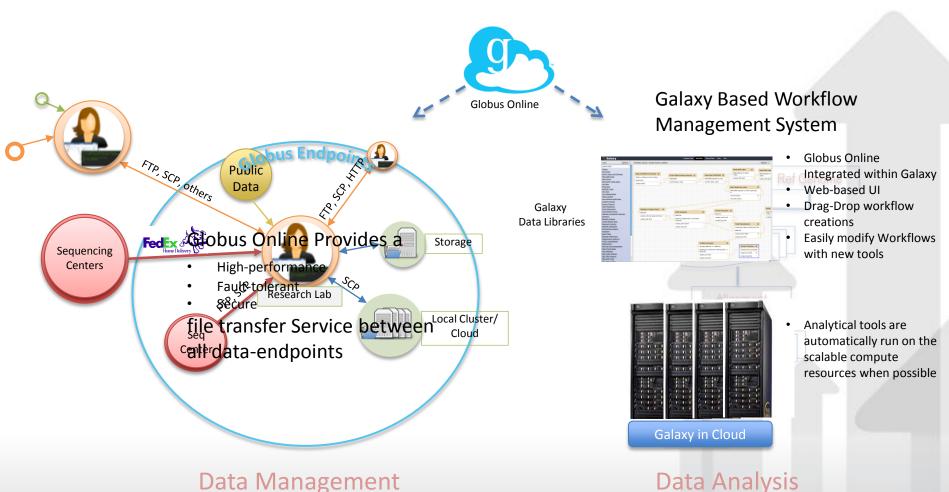
What can KBase do?







Genomics Analysis using Globus Online and Galaxy



Data Analysis

www.globusonline.org



Thank you!