CIPRES Cyberinfrastructure for Phylogenetic Research

The CIPRES Science Gateway: A Community Resource for Phylogenetic Analyses

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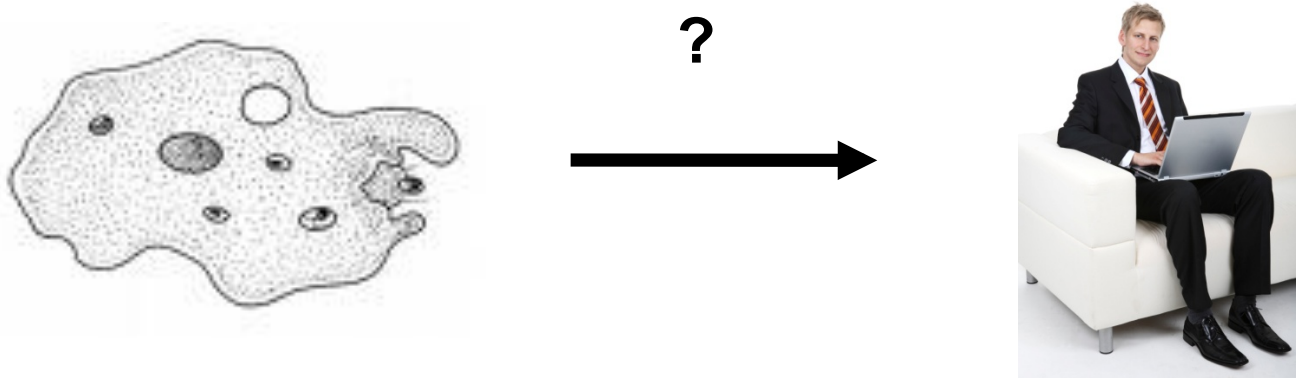
San Diego Supercomputer Center

POWERED BY TeraGrid

SDSC

Systematics is the study of biological diversity and its origins. It focuses on understanding evolutionary relationships among organisms.



Originally, evolutionary relationships were inferred from morphology alone:

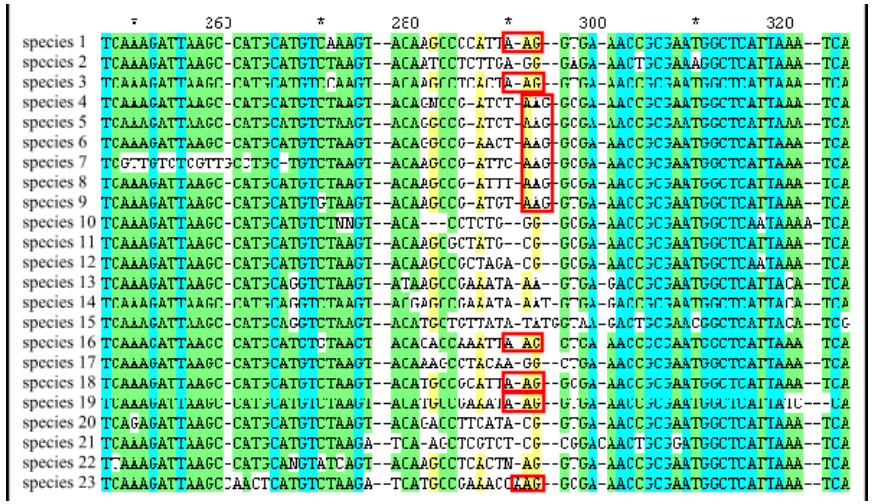
Morphological characters are scored “by hand” to create matrices of characters.

Scoring occurs via low volume/low throughput methodologies

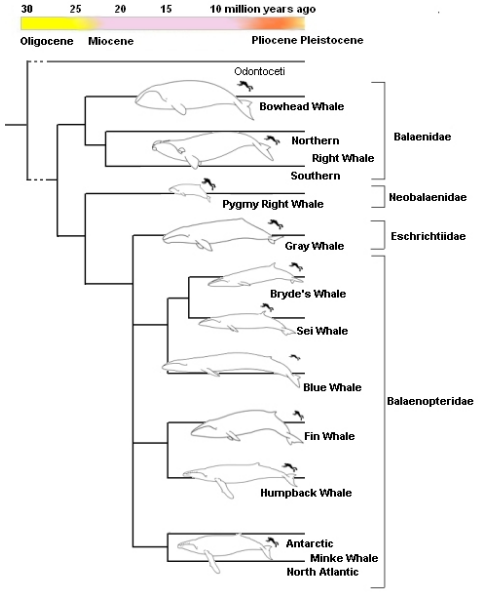
Even though tree inference is NP hard, matrices created using morphological characters alone are typically relatively small, so computations are relatively tractable (with heuristics developed by the community)

Evolutionary relationships are now inferred from DNA sequence comparisons:

Align sequences to determine evolutionary equivalence:



Infer evolutionary relationships based on some set of assumptions:



Inferring Evolutionary relationships from DNA sequence comparisons is powerful:

DNA sequences are determined by fully automated procedures.

Sequence data can be gathered from many species at scales from gene to whole genome.

The high speed and low cost of NexGen Sequencing means new levels of sensitivity and resolution can be obtained.

Inferring Evolutionary relationships from DNA sequence comparisons is powerful, BUT:

Current analyses often involve 1000's of species and 1000's of characters, creating very large matrices.

Sequence alignment and Tree inference are NP hard, so even with heuristics, computational power often limits the analyses (already).

The length of tree search analysis scales exponentially with number of taxa and with number of characters with codes in current use.

There are at least 10^7 species, each with 3000 - 30,000 genes, so the need for computational power and new approaches will continue to grow.

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The CIPRES Project was created to support this new age of large phylogenetic data sets. The project had as its principal goals:

1. **Developing heuristics and tools for analyzing the large DNA data sets that are available.**

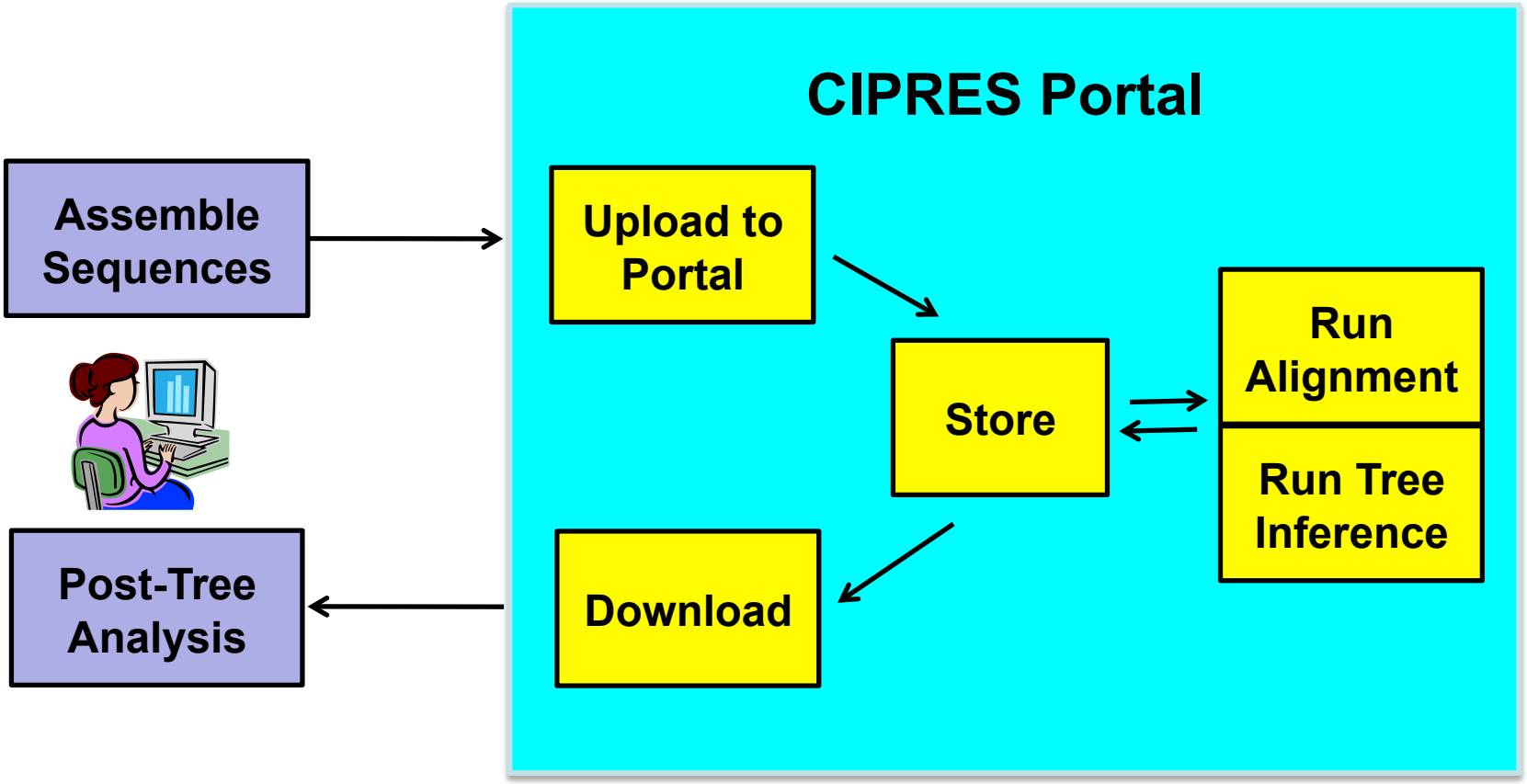
2. **Improving researcher access to computational resources.**

The CIPRES Portal was designed to allows users analyze large sequence data sets using community codes on a significant computational resource.

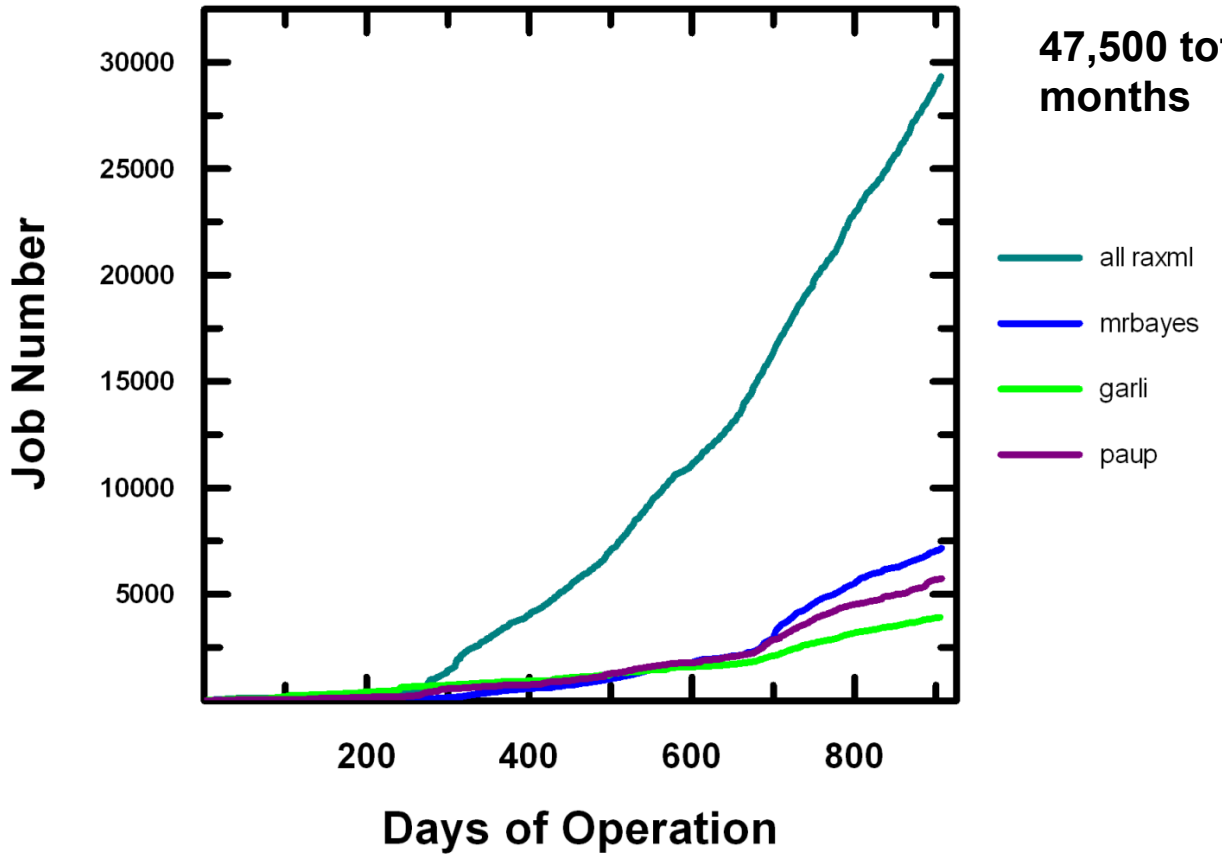
The CIPRES Portal provided:

- **Login-protected personal user space for storing results indefinitely.**
- **Access to most/all native command line options for each code.**
- **Support for adding new tools and new versions as needed.**

Workflow for the CIPRES Portal:



Usage Statistics for CIPRES Portal 5/2007 – 11/2009



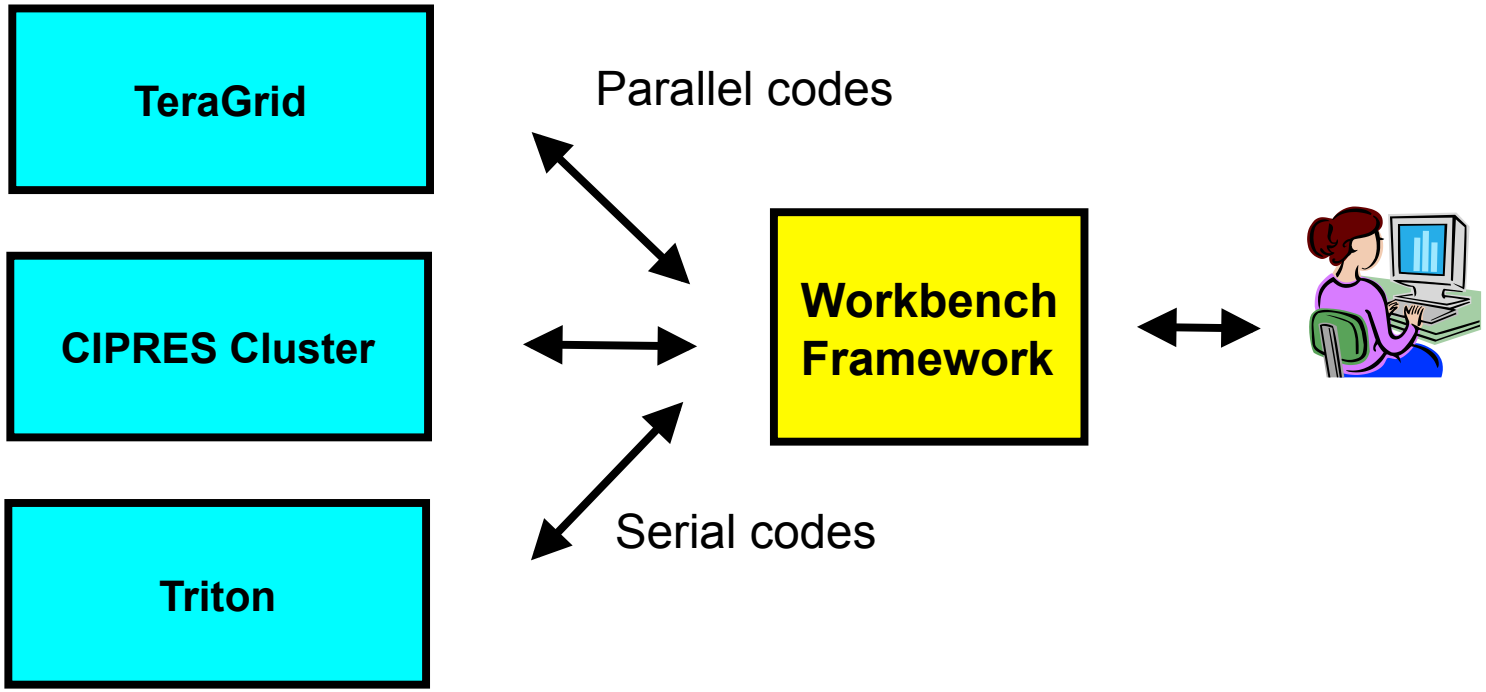
47,500 total jobs in 30 months

Limitations of the original CIPRES Portal

- all jobs were run serially (efficient, but no gain in wall time)
- runs were limited to 72 hours
- demand for job runs was increasing
- the cluster was modest (16 X 8-way dual core nodes)
- the cluster was at the end of its useful lifetime
- funding for the project was ending

This is not a scalable, sustainable solution!

The solution: make community codes available on scalable, sustainable resources via Science Gateway Program



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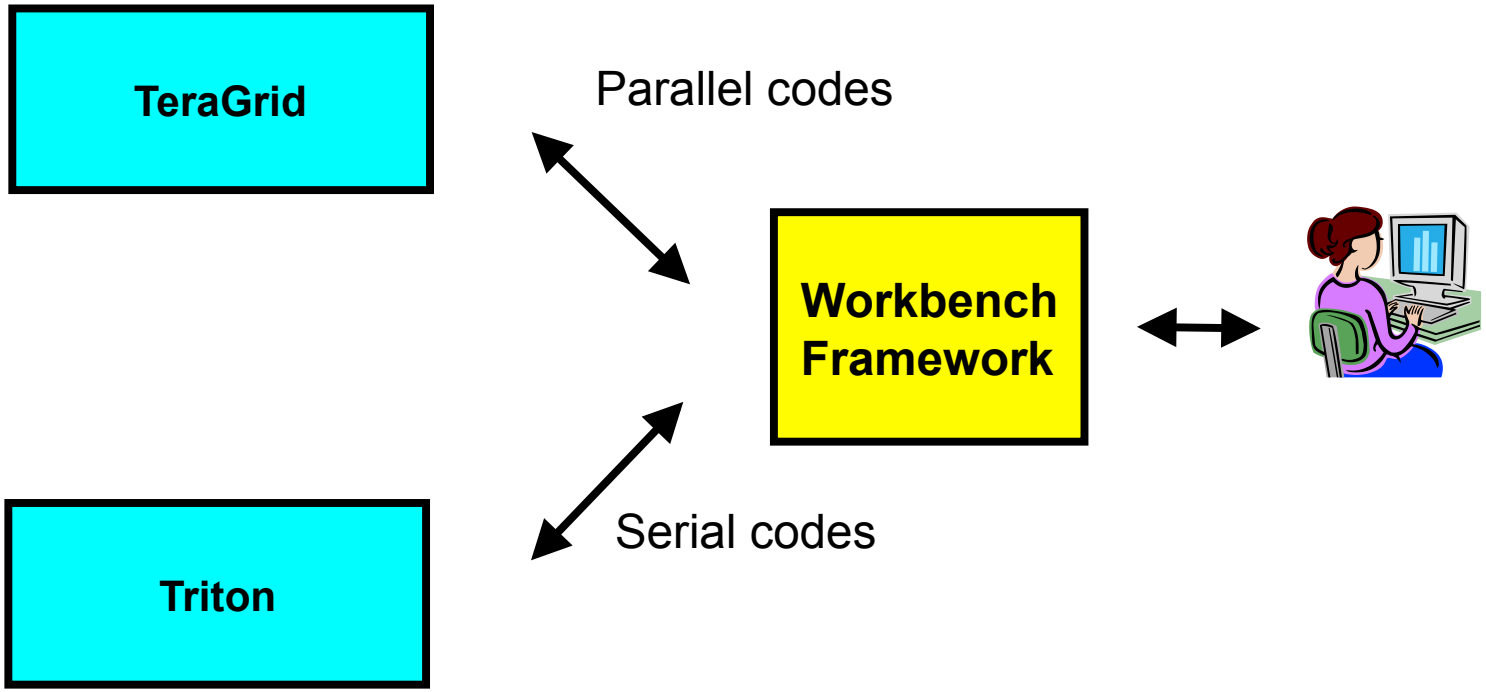


Greater than 90% of all computational time was used for three tree inference codes: MrBayes, RAxML, and GARLI.

Deploy parallel versions of these codes on TeraGrid Machines; initially using Globus/GRAM.

Work with community developers to improve the speed-up available through the parallel codes offered by CSG.

Add new parallel codes (e.g. MAFFT) as they appear in the community.

Keep other serial codes on local SDSC resources that provide the project with fee-for-service cycles.

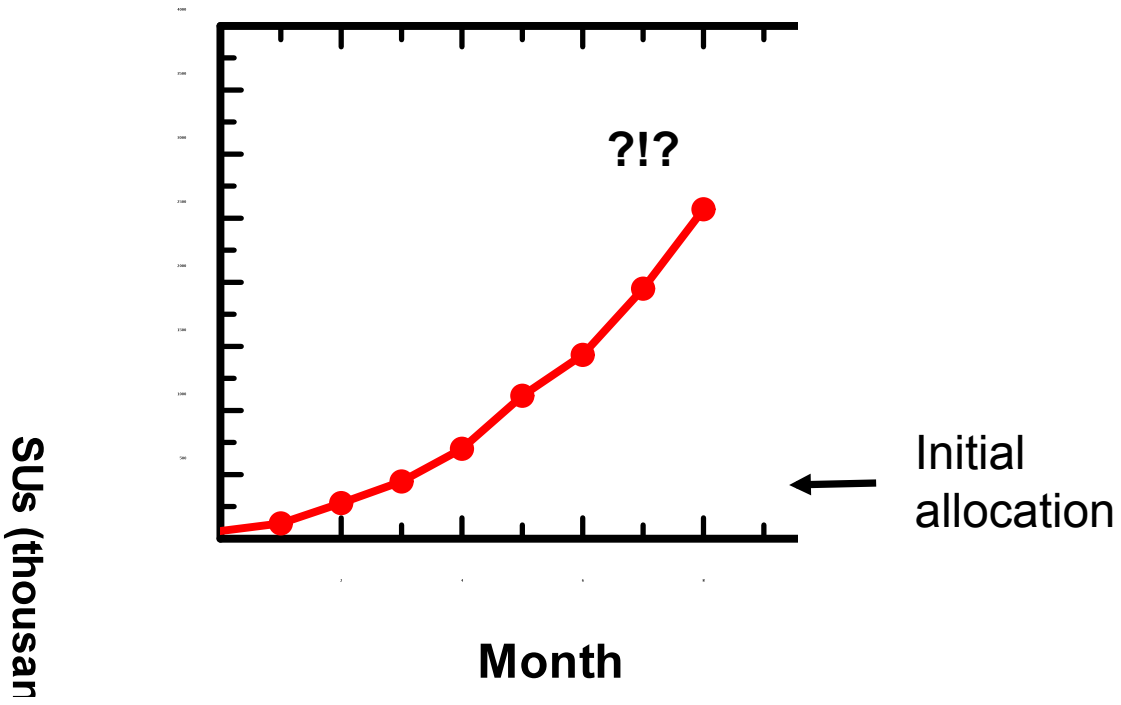
CIPRES Science Gateway Code Improvements

- Hybrid MPI/Pthreads version of RAxML was developed
- Hybrid MPI/OpenMP version of MrBayes was developed
- Single-node runs are more efficient than before
- Multi-node runs with more cores are possible
  - Scalability before was limited to about 8 cores for typical analyses
  - Codes now scale well to 10s of cores for typical analyses

Parallel code profiles on Trestles

Code	Type	Max cores	Speed-up	Efficiency
MrBayes	Hybrid MPI/OpenMP	32	2.4 X (1 nodes)	~60%
RAxML	Hybrid MPI/Pthreads	60	3.0 X (2 nodes)	~ 60%
GARLI	MPI	100	77 X (100 nodes)	77-94%
MAFFT	Pthreads	32	10 X	25%

What happens if you build it and too many people come???



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Job Attrition on the CIPRES Science Gateway*

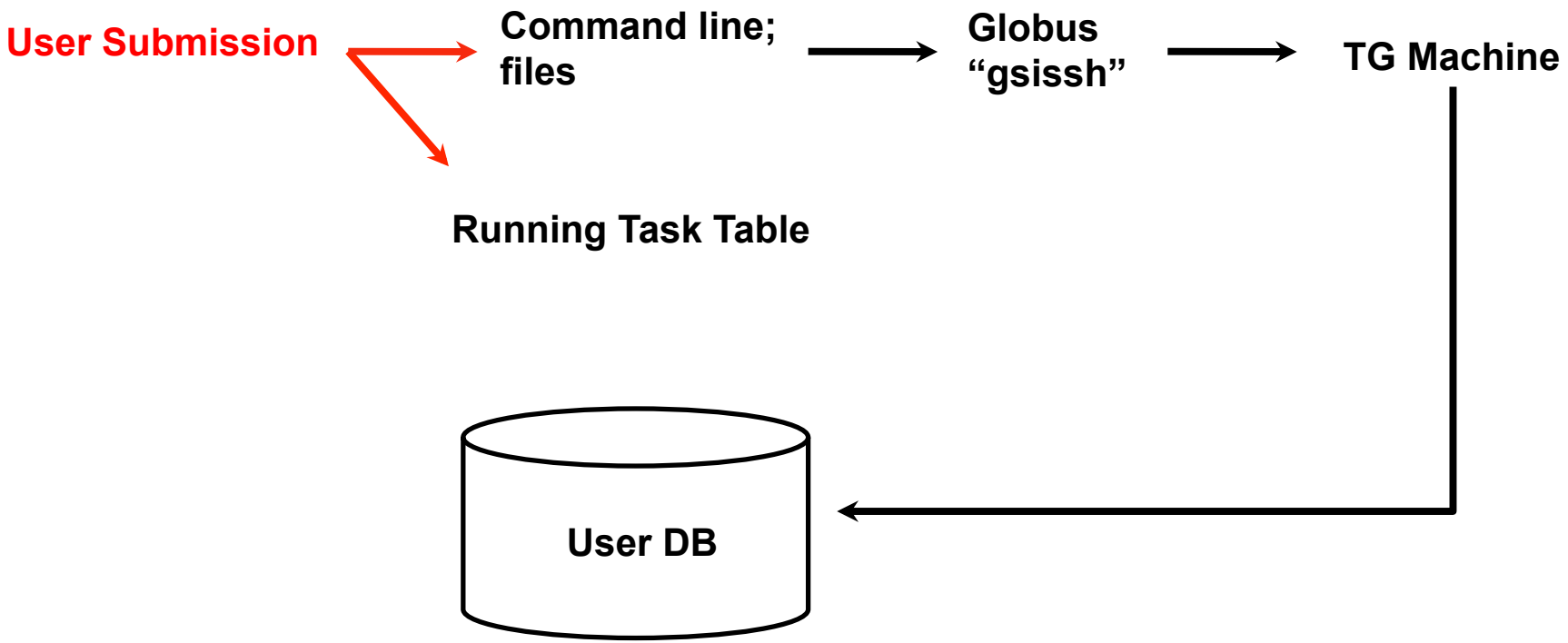
*March – August 2010

Error Impact analysis

	CPU time	User	Staff
Input error	0	med	low
Machine error	0	med	low
Communication error	high	high	high
Unknown error	?	med	low

CONCLUSION: Time to refactor the job monitoring system!

Normal Operation



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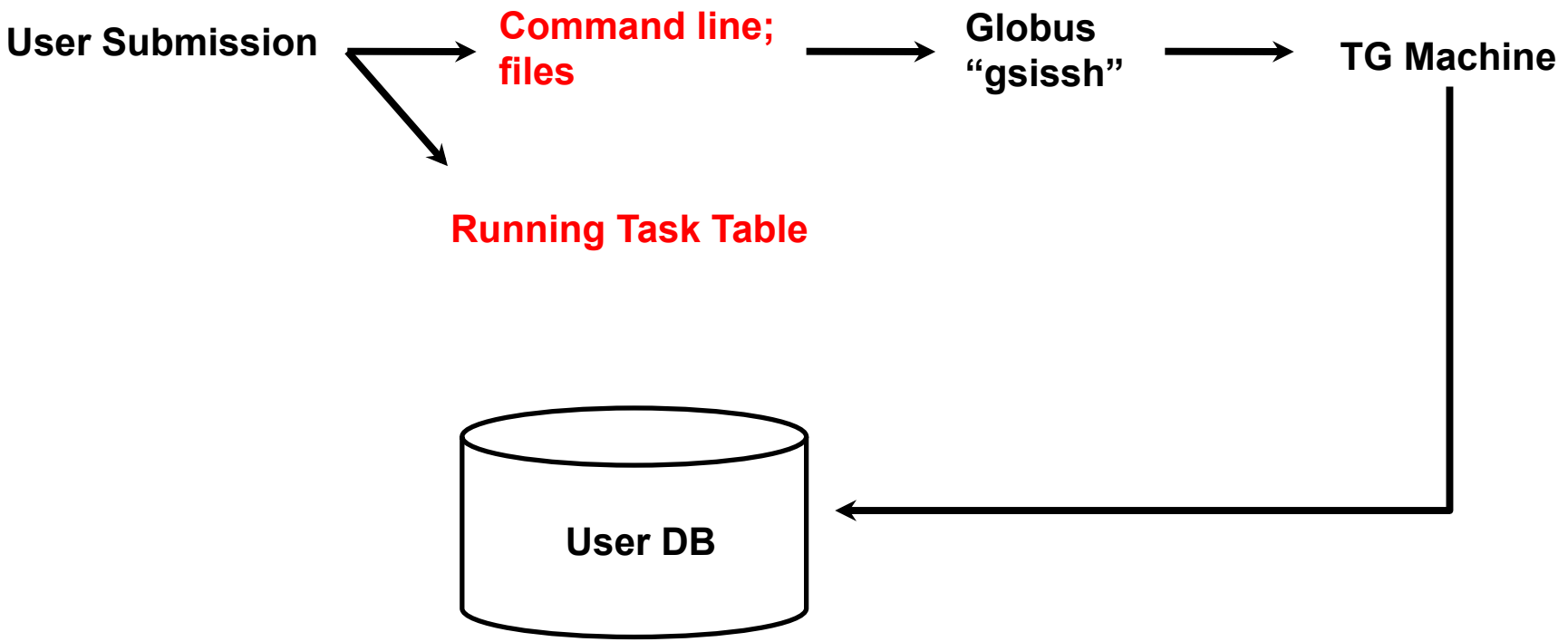

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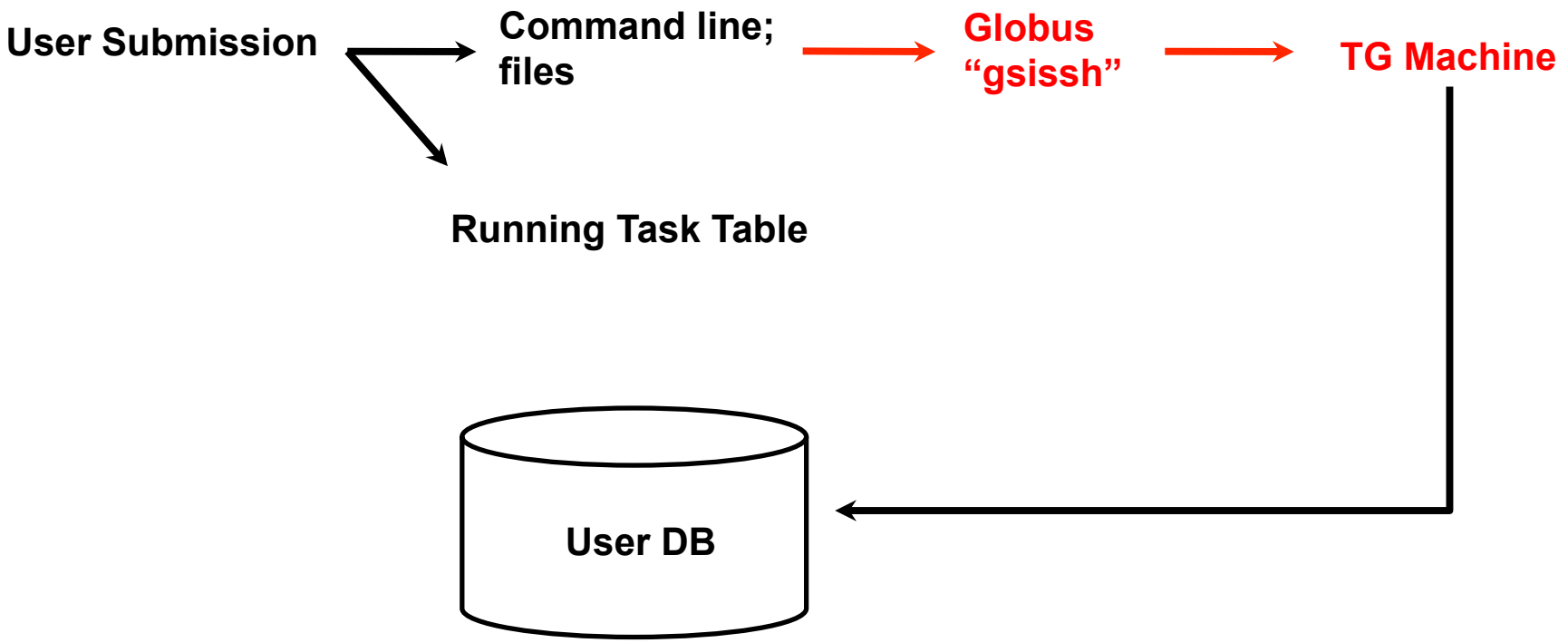

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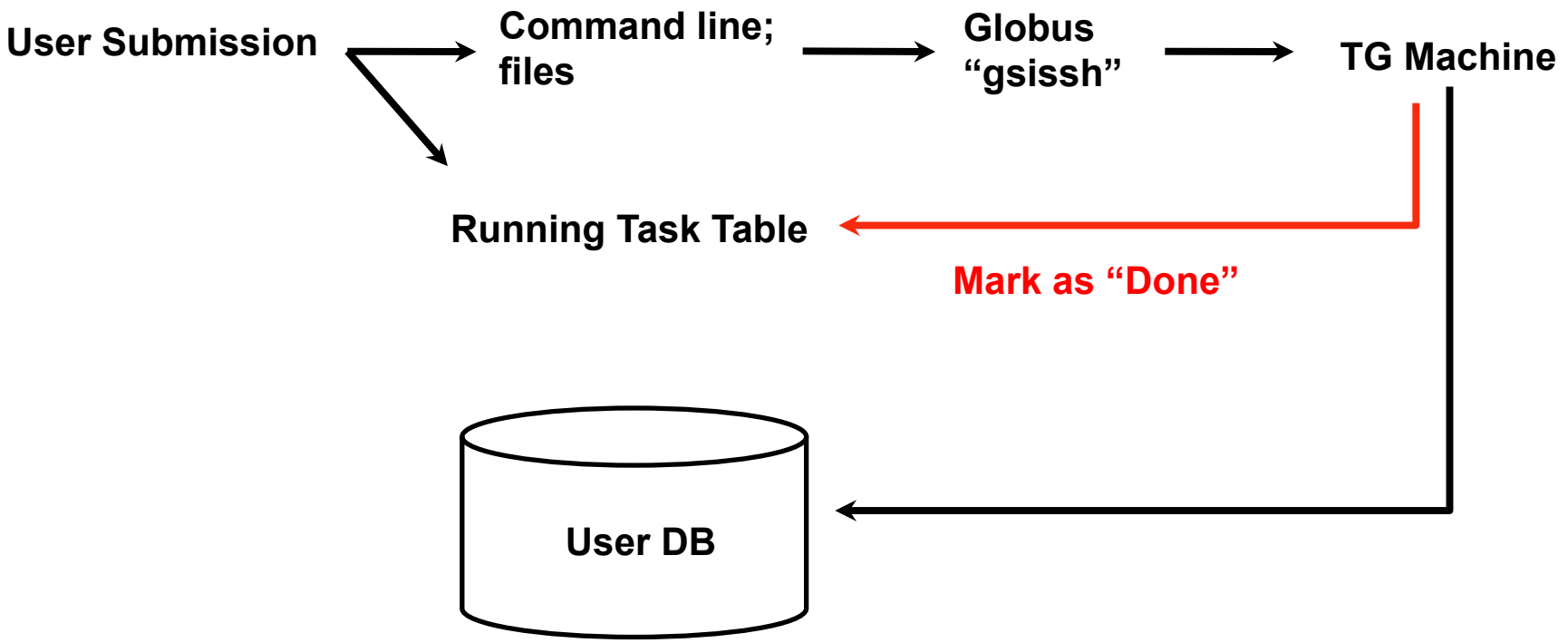

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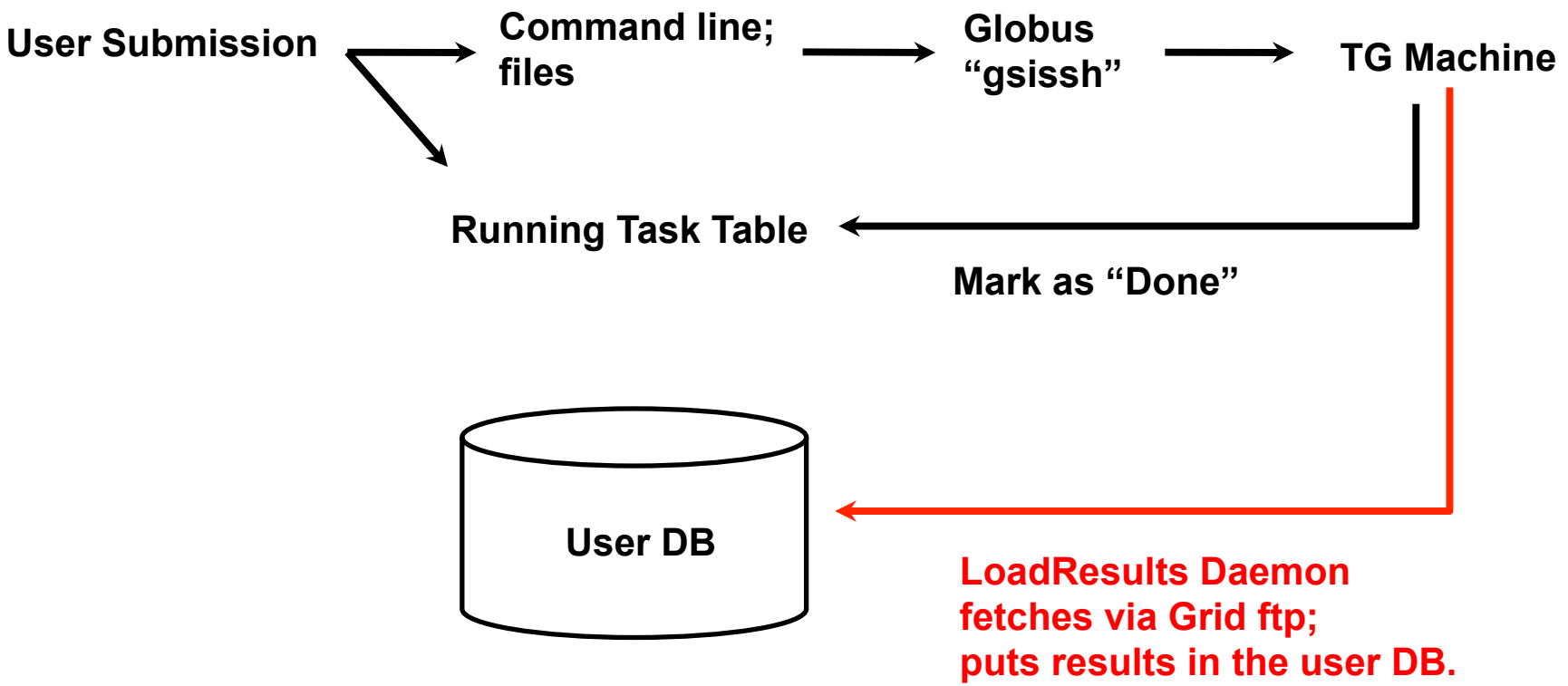

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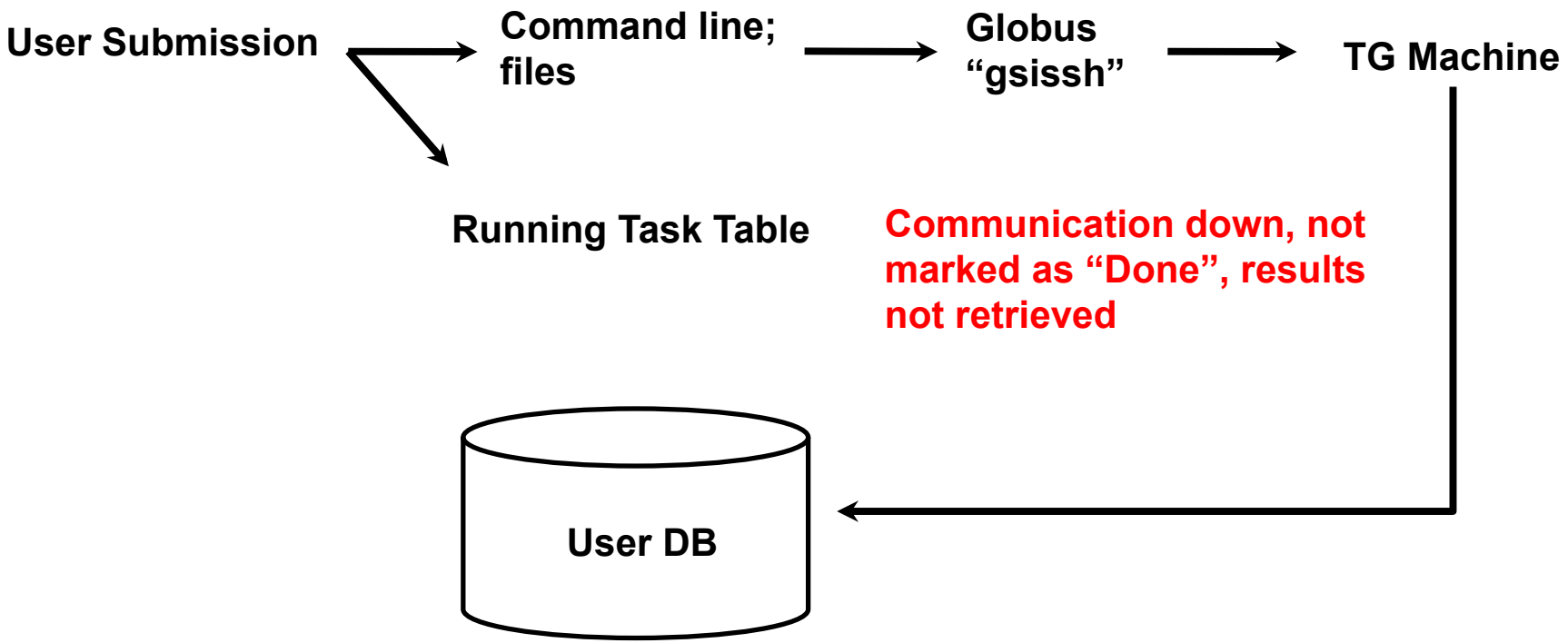

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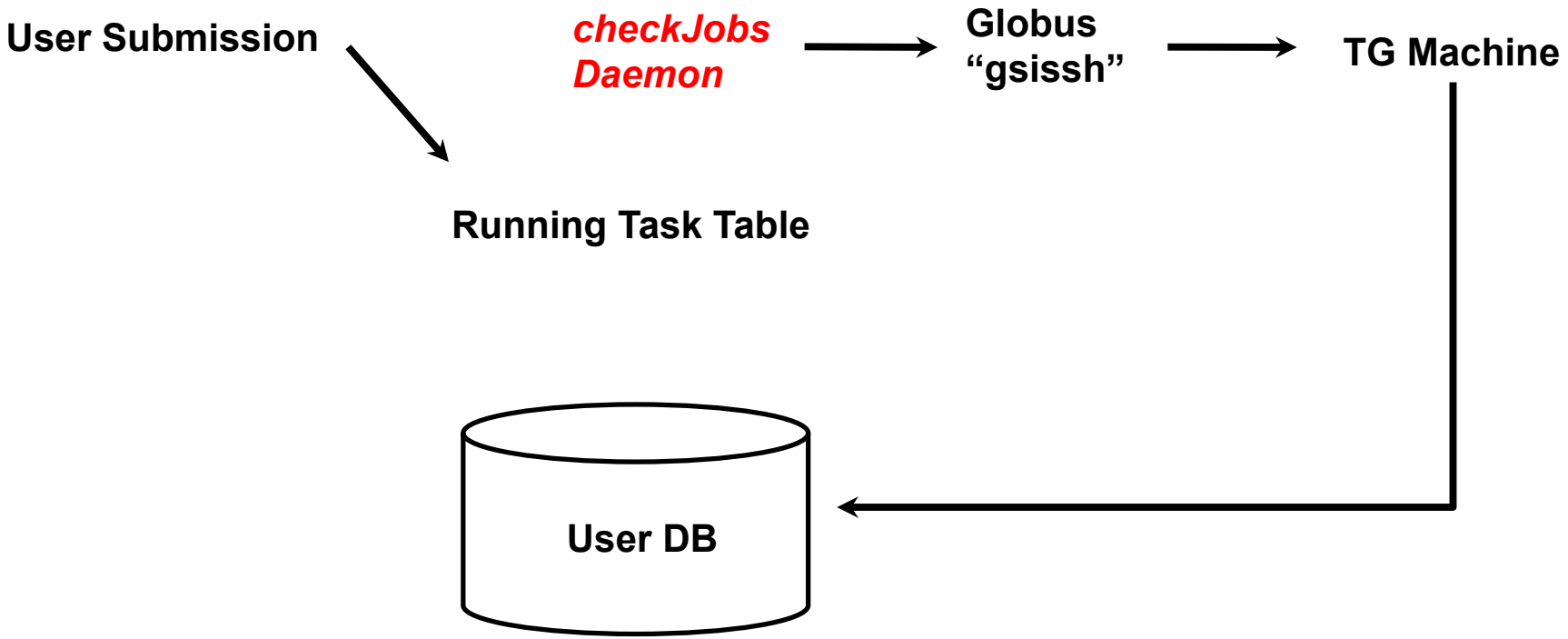

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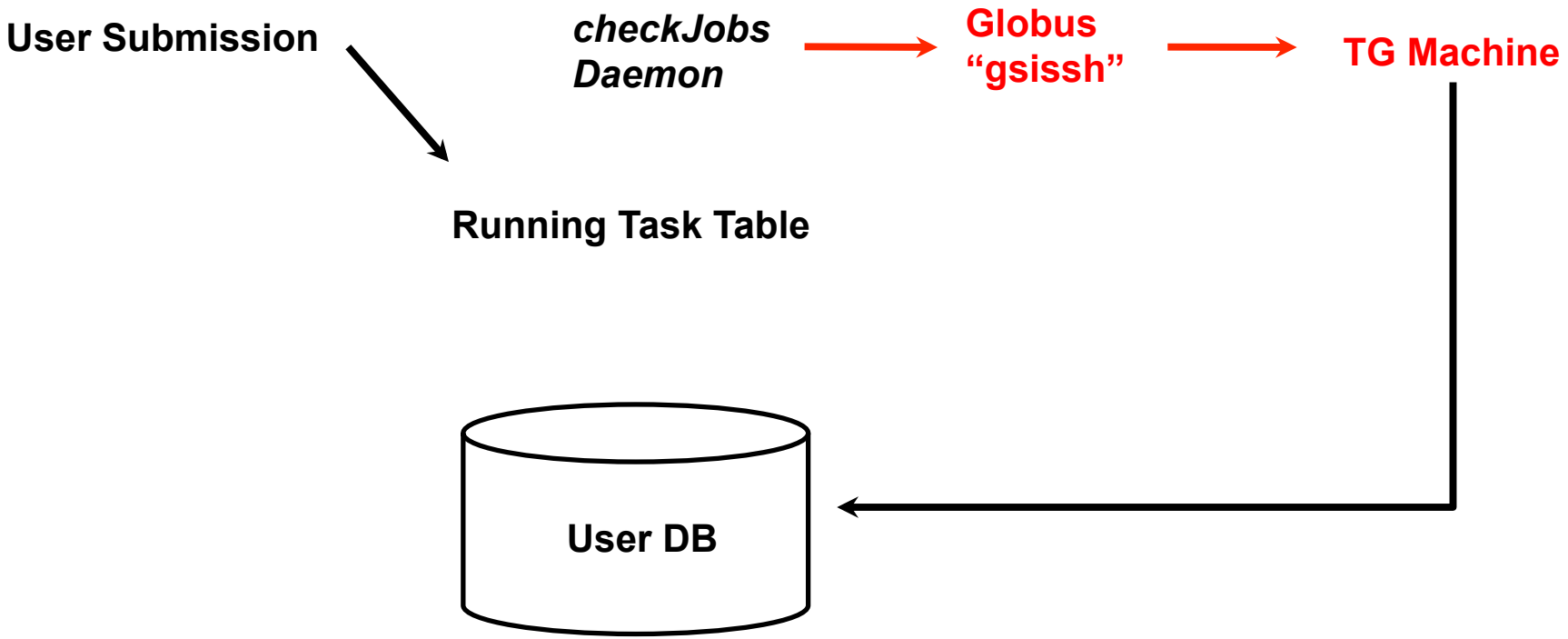

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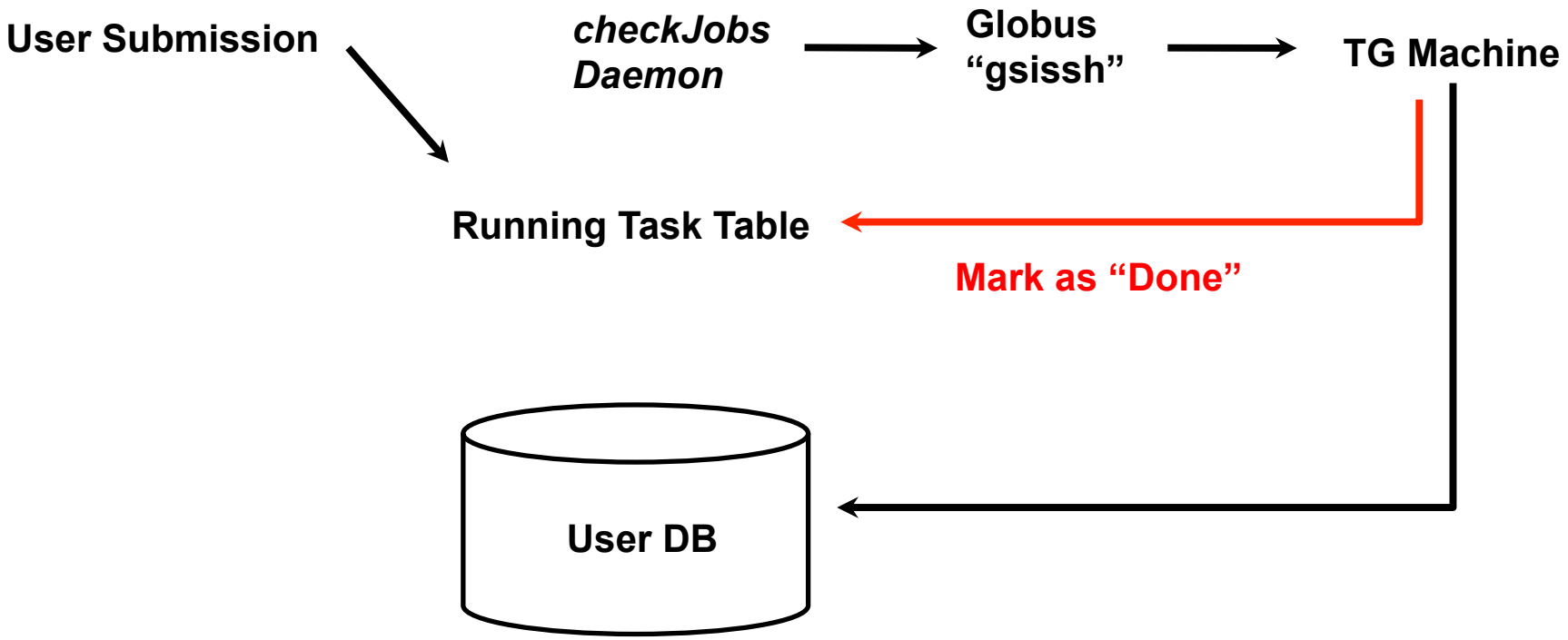

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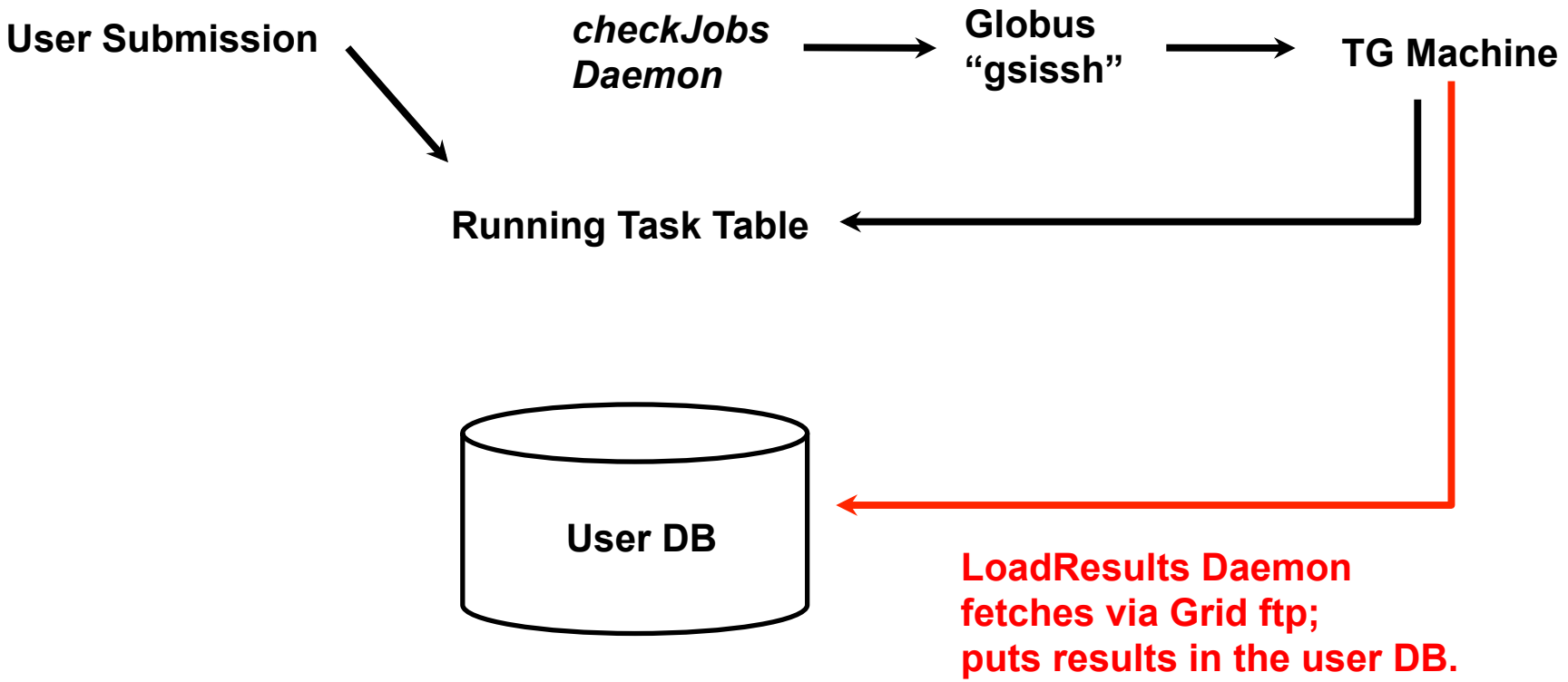


Jobs Saved by the GSISSH / Task Table System

	SEPT	OCT
Jobs Saved	159*	266*

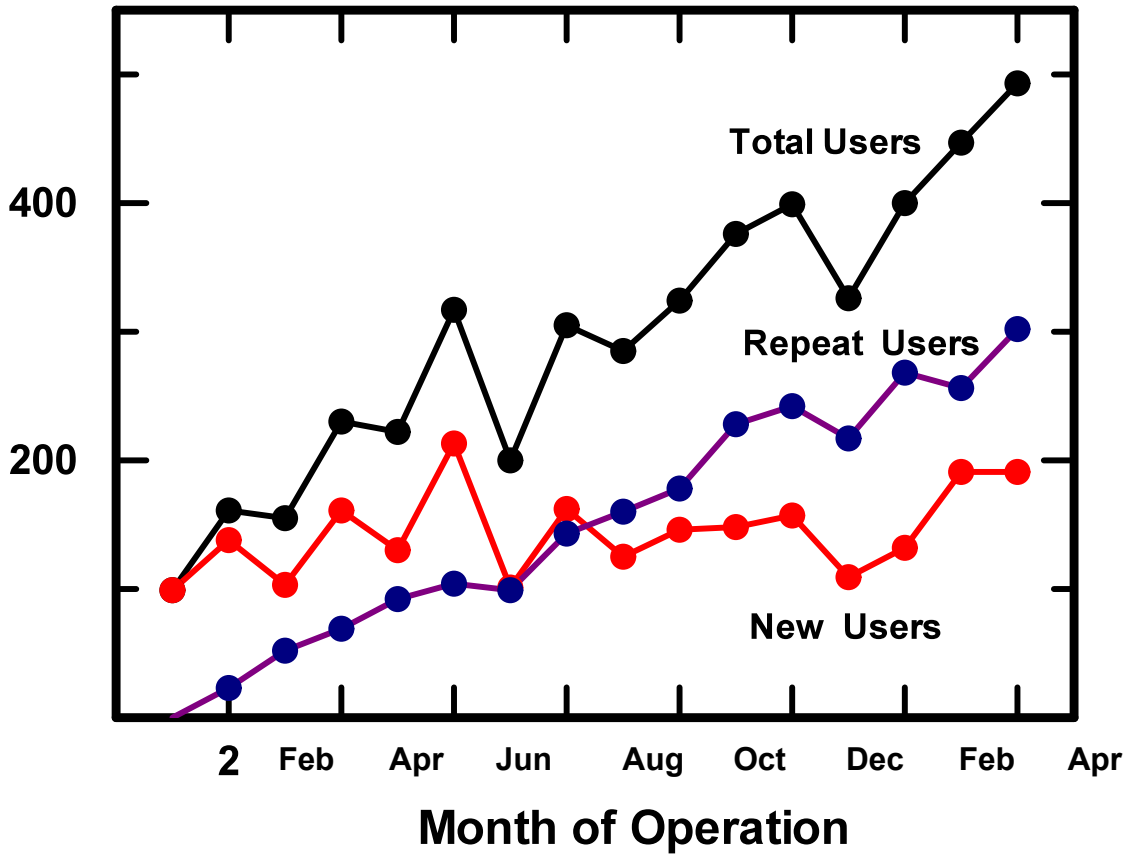
* 7% of all submitted jobs

What happens if you build it and too many people come???

- **make sure resource use is efficient**
- **make sure resource use delivers impact**
- **implement policies to maximize access for all**

Make sure resource use delivers impact: Usage and Outcomes

CIPRES Science Gateway Usage Dec 2009 – April 2011



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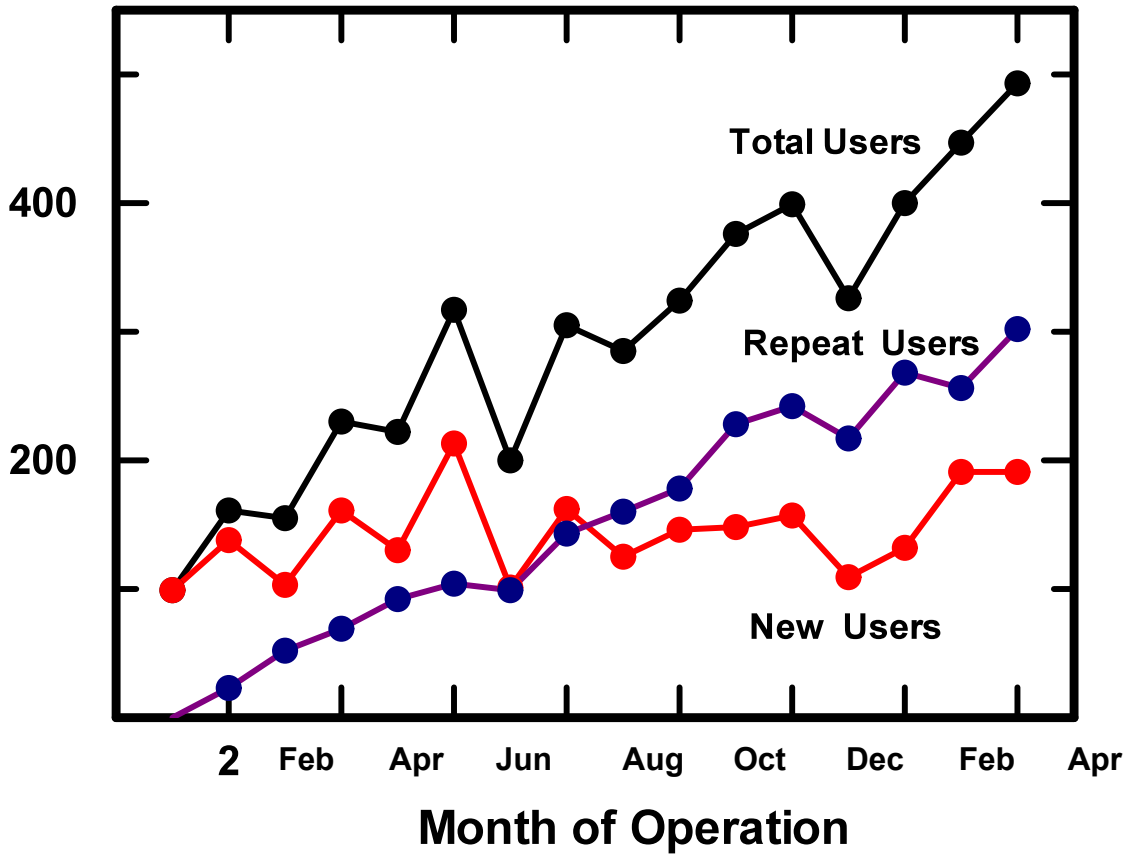

4X increase in users/month

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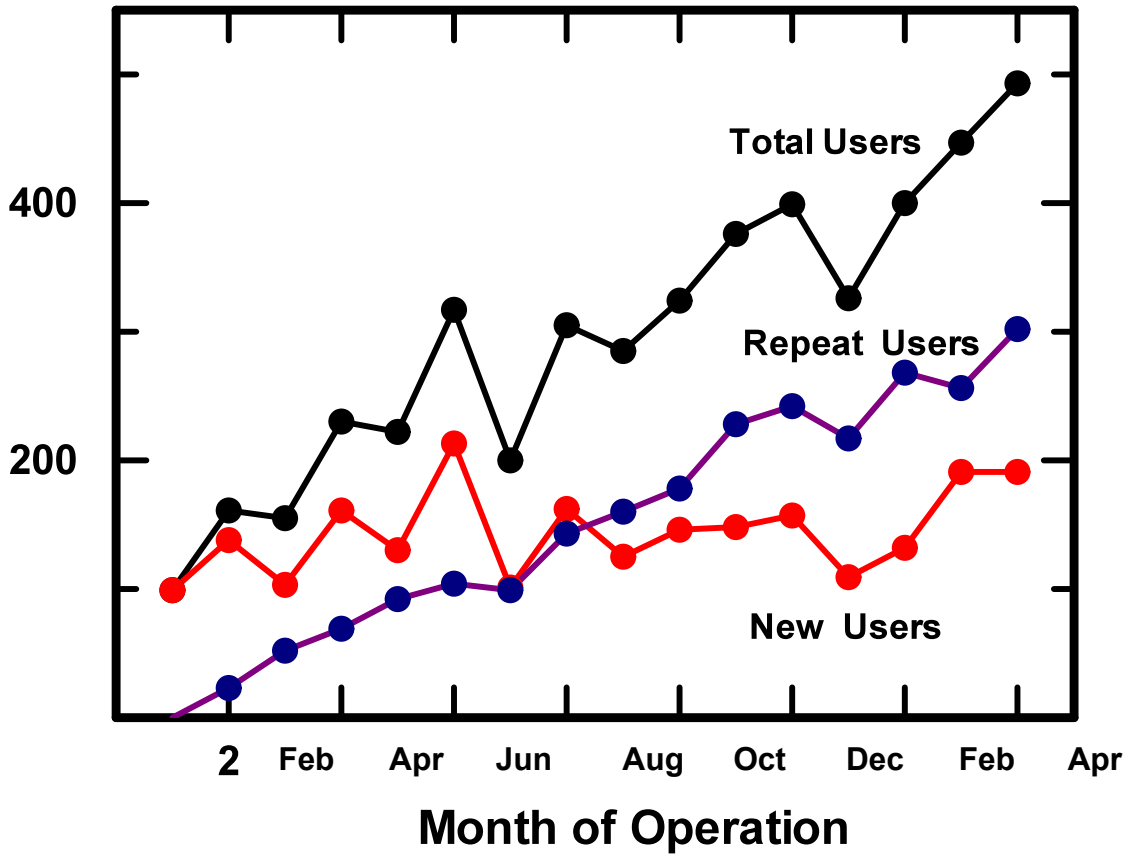

4X increase in users/month

2456 new TG users

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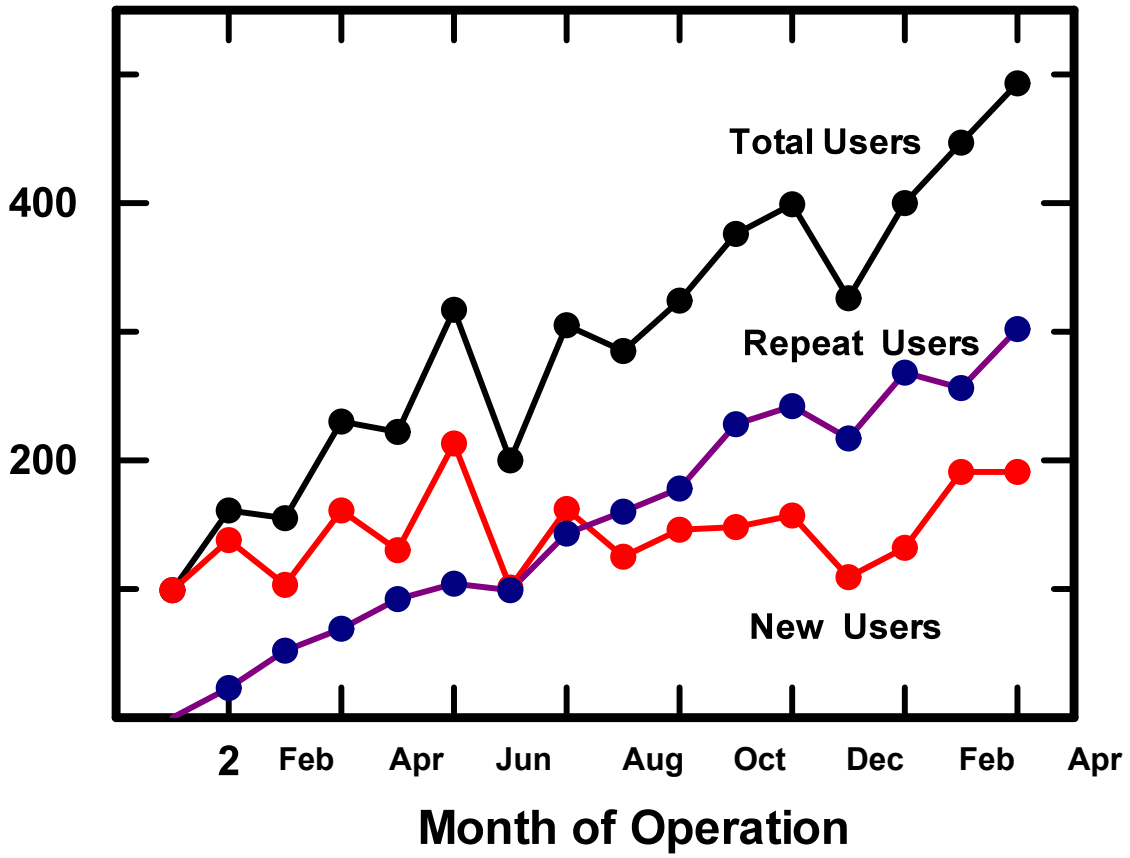

4X increase in users/month

2456 new TG users

At least 100 new TG users in each month

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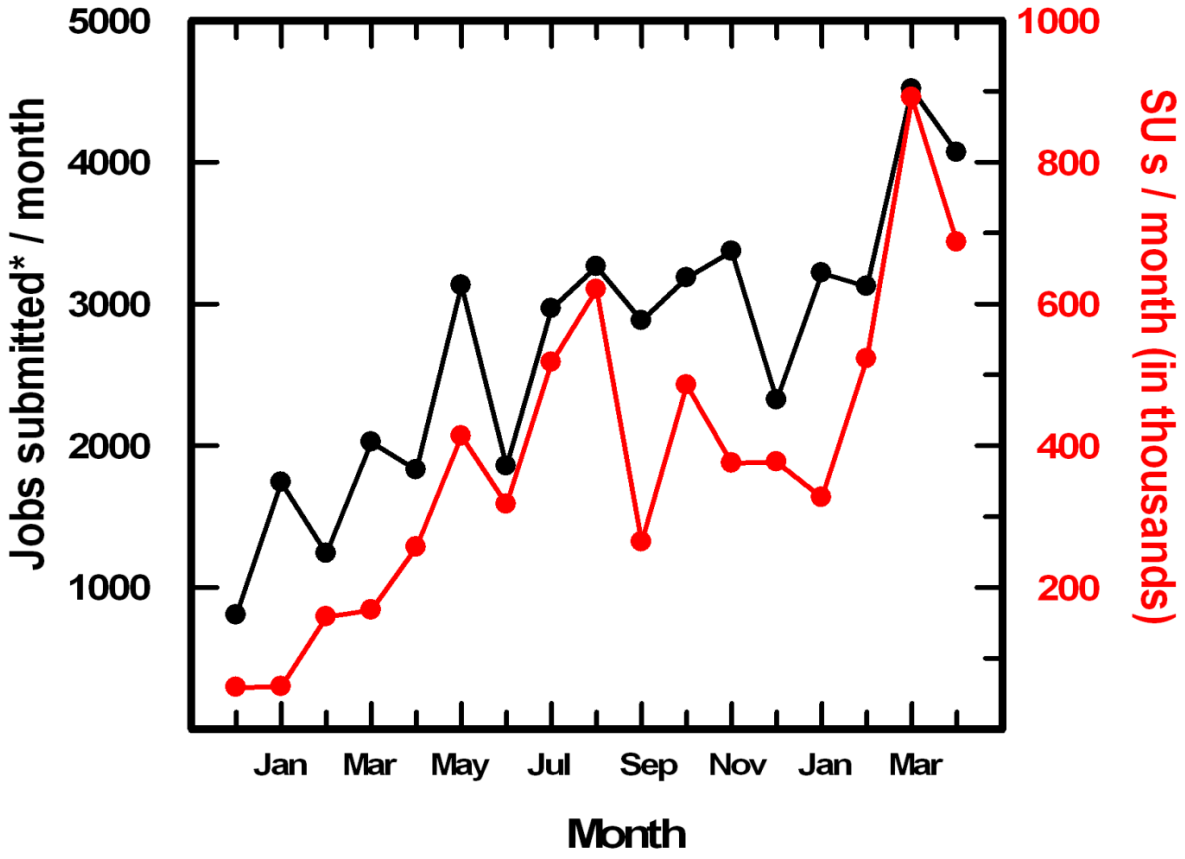

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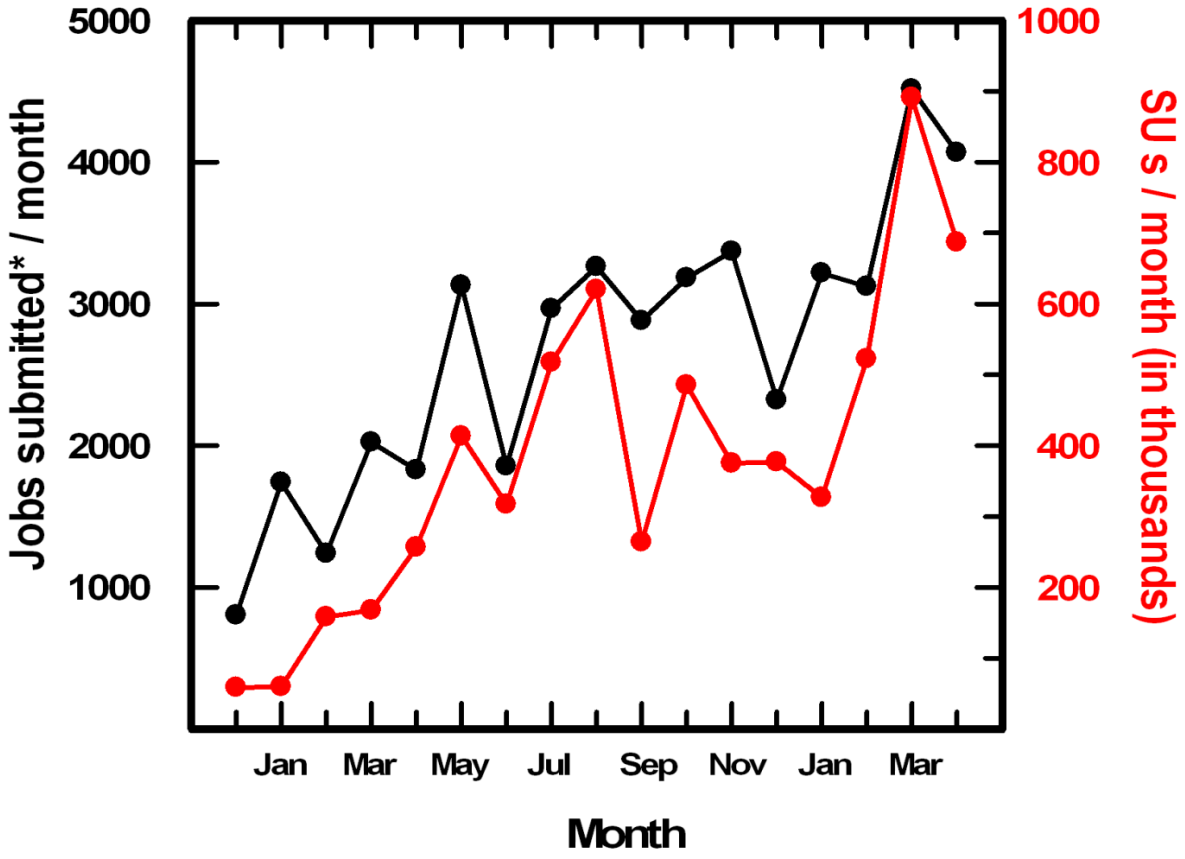

4-fold increase in jobs submitted /month

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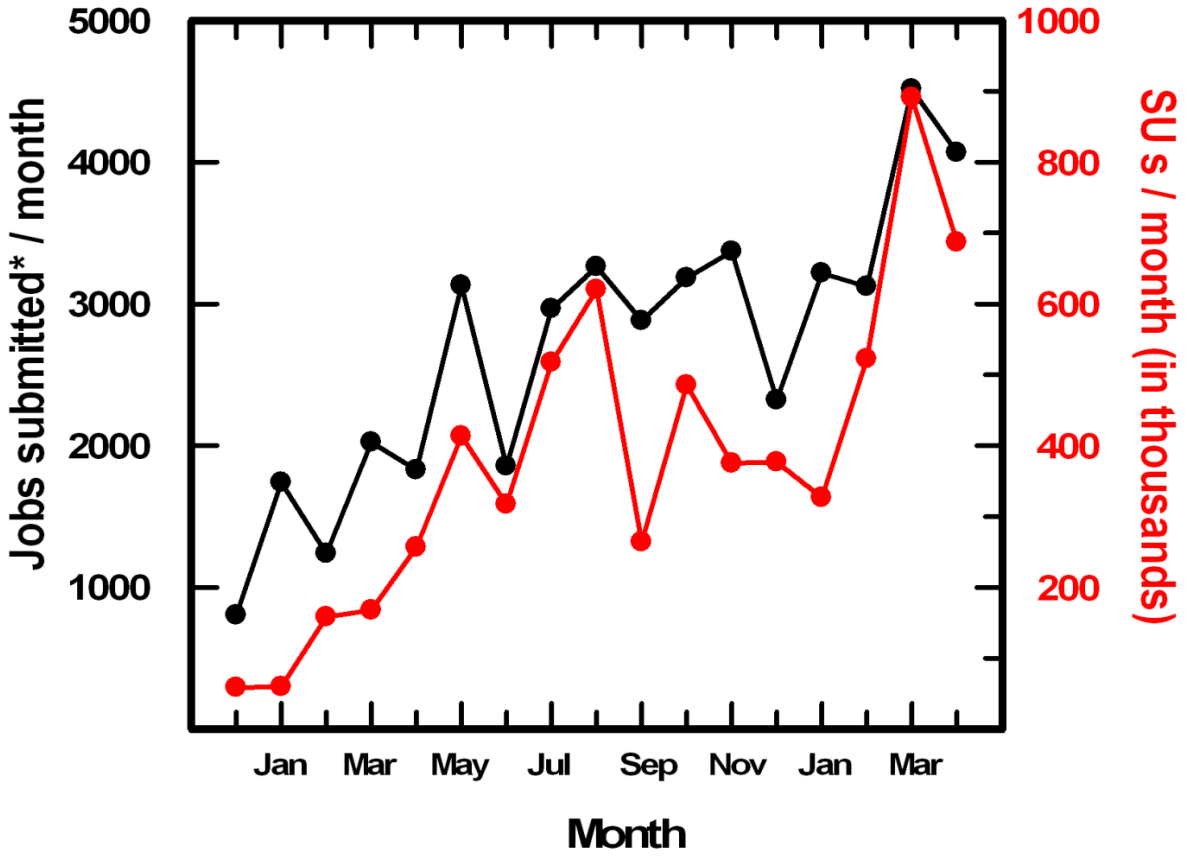

4-fold increase in jobs submitted /month

10+ fold increase in SUs/month

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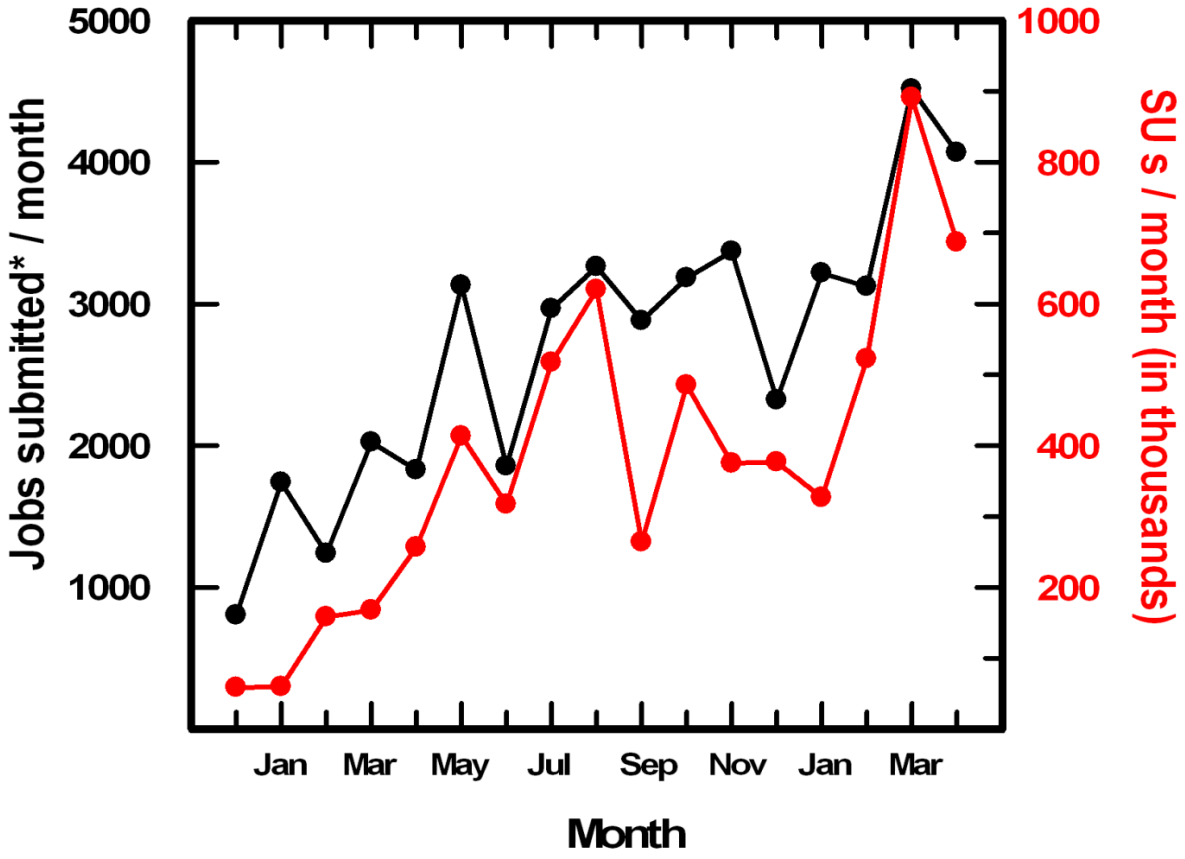


4-fold increase in jobs submitted /month

10+ fold increase in SUs/month

45,500 total job submissions in 17 months

Intellectual Merit:

Publications enabled by the CIPRES Science Gateway/CIPRES Portal:

Year	Number
2011*	38
2010	74
2009	56
2008	4

*As of April 1, 2011

Publications in the pipeline:

Status	Number
In preparation	103
In review	24

Intellectual Merit:

"…quick and reliable results often help with brainstorming and pushing 'things into the right direction.' The service is invaluable."

Broad Impact:

- **Used for curriculum delivery by at least 57 instructors.**
- **Jobs run for researchers in 23/29 EPSCOR states.**
- **Routine submissions from Harvard, Berkeley, Stanford…..**
- **76% of users are in the US or have a collaborator in the US**
- **In Q1, 2011, 28% of all TG users who ran jobs ran them from the CSG**

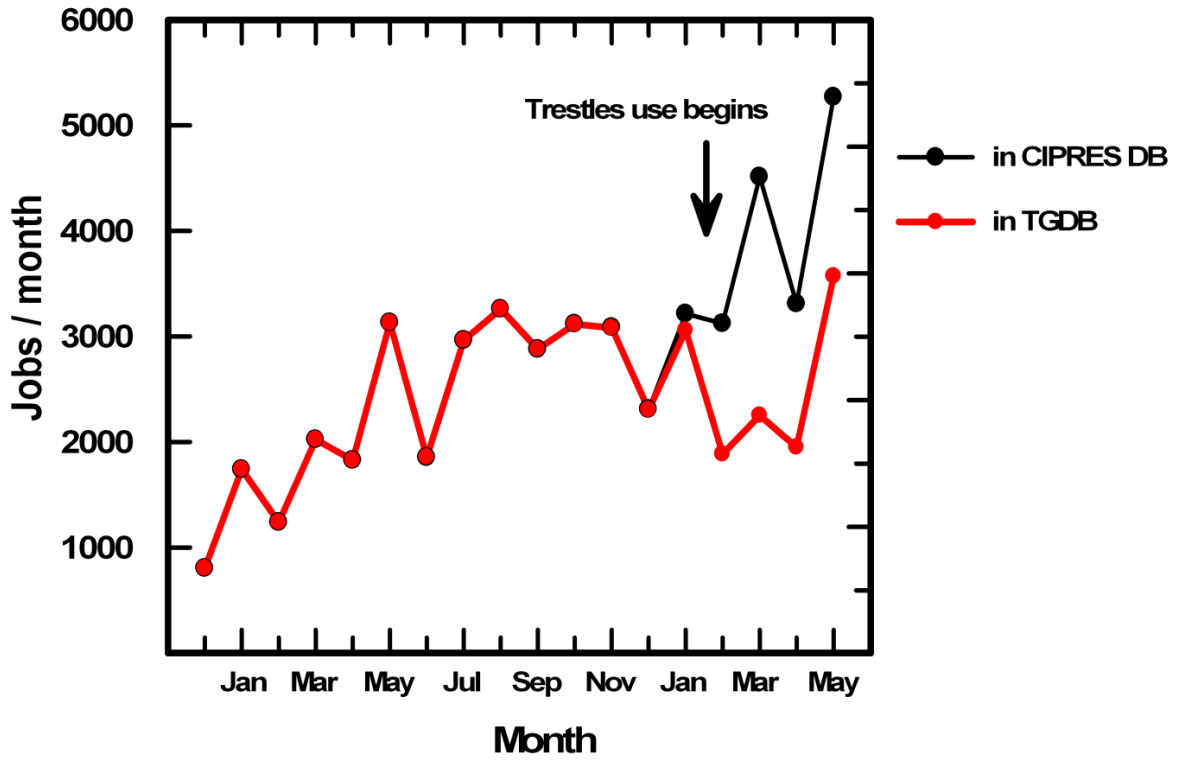
Broad Impact:

“The wall time for these data sets are 30 min (2000 BS reps) [on the CSG], but locally it would take 24 hours for each run. So, instead of 10 days to complete all the analyses with a few local computers, I have publication quality trees overnight.”

Make sure resource use delivers impact: Usage and Outcomes

We know how many jobs are *submitted*, how many of these jobs produce useful outcomes?

Not All Job Submissions to *Trestles* Appear in the TGDB



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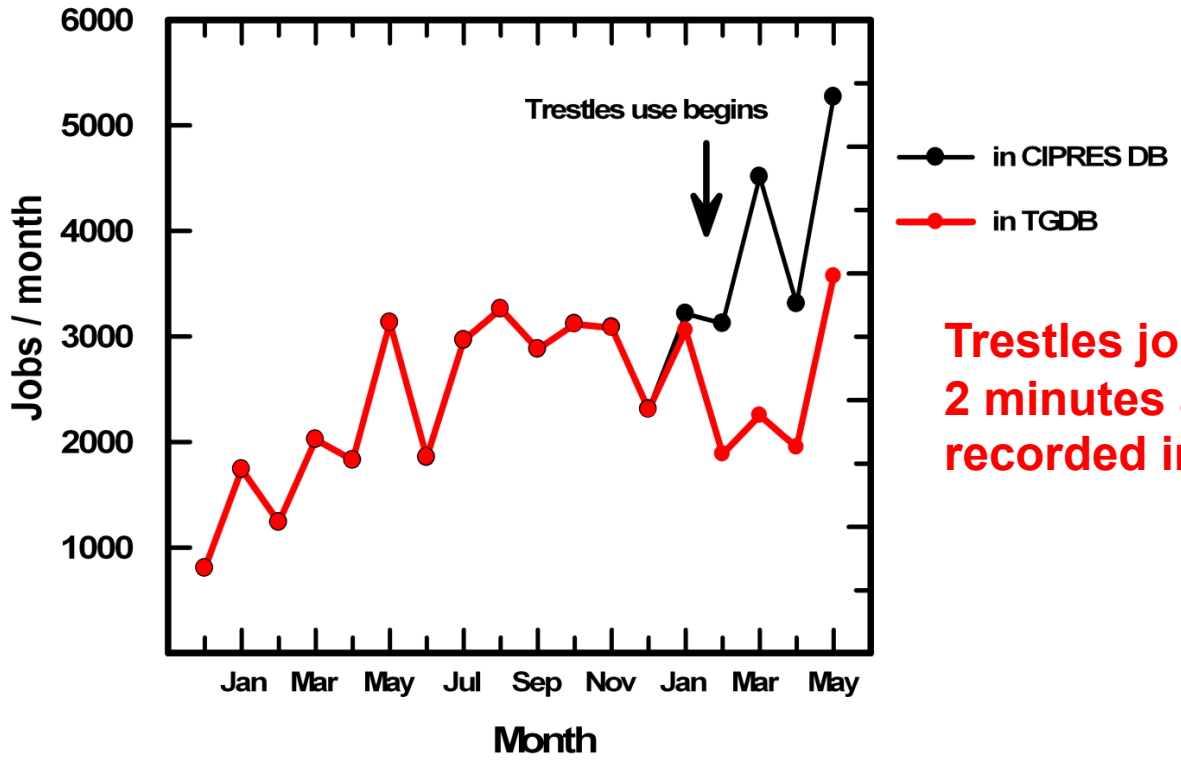

Trestles jobs less than 2 minutes are not recorded in TGDB

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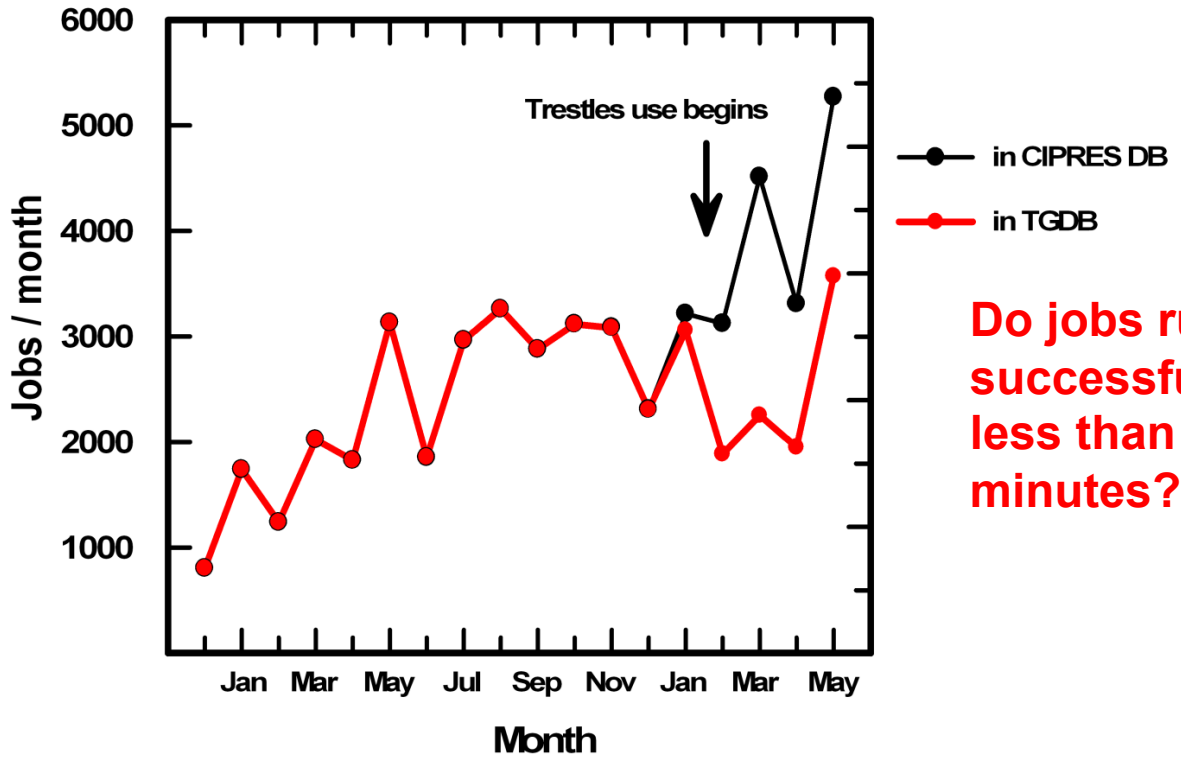

Do jobs run successfully in less than 2 minutes?

Categorization of RAxML and MrBayes jobs by outcome and duration*

	RAxML		MrBayes	
	Jobs	Fraction	Jobs	Fraction
Failed	885	0.394	257	0.230
Succeeded	1363	0.606	860	0.770
< 2 minutes	521	0.232	18	0.016
≥ 2 minutes	842	0.375	842	0.754

* Jobs run between 3/16/2011 and 4/17/2011.

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Categorization of CSG users by job outcome and duration *

	Users	Fraction
Only Failed	50	0.13
Run Succeeded	345	0.87
Only < 2 minutes	61	0.15
≥ 2 minutes**	284	0.72

*Jobs between 3/17/2011 and 4/17/2011

** The user ran at least one job that produced results and recorded an SU charge.

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15% of all users only submitted short jobs

*Jobs between 3/17/2011 and 4/17/2011

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≥ 2 minutes**	284	0.72

13% of all users did not submit a successful job

*Jobs between 3/17/2011 and 4/17/2011

** The user ran at least one job that produced results and recorded an SU charge.

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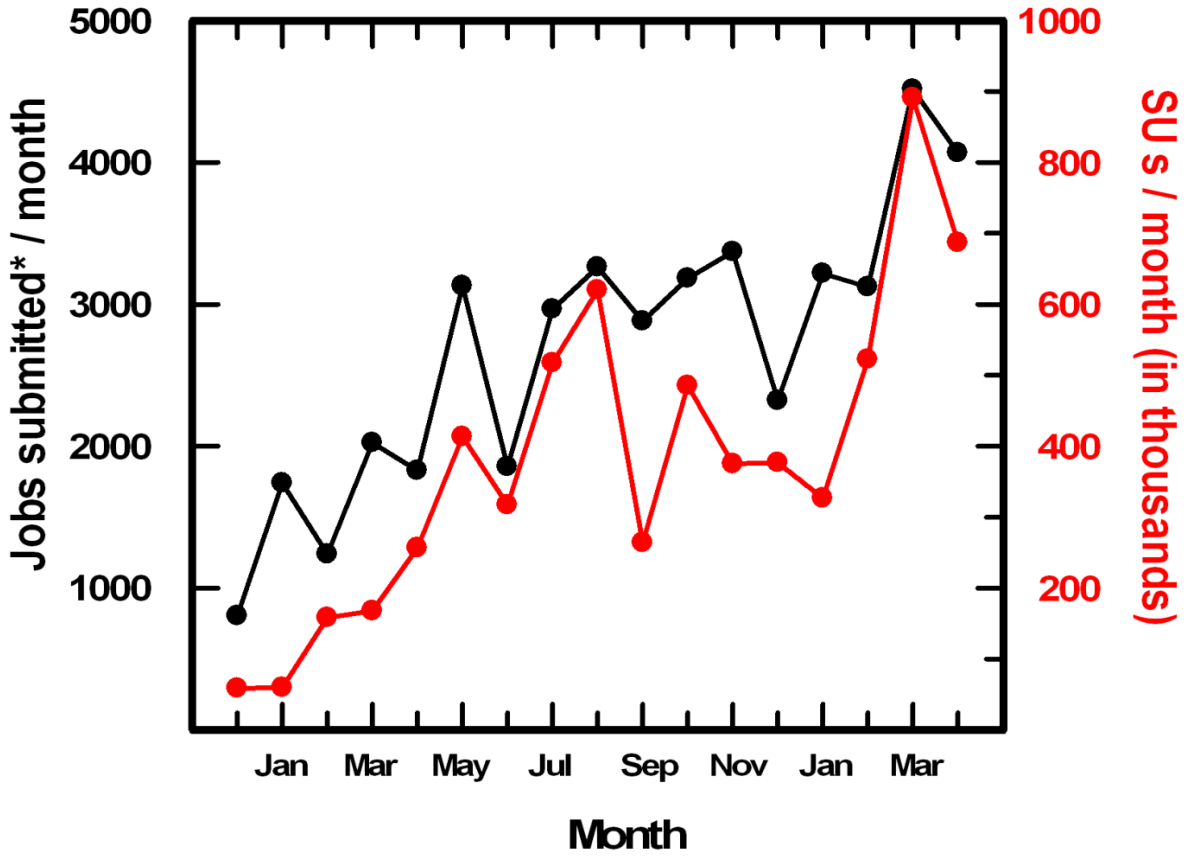
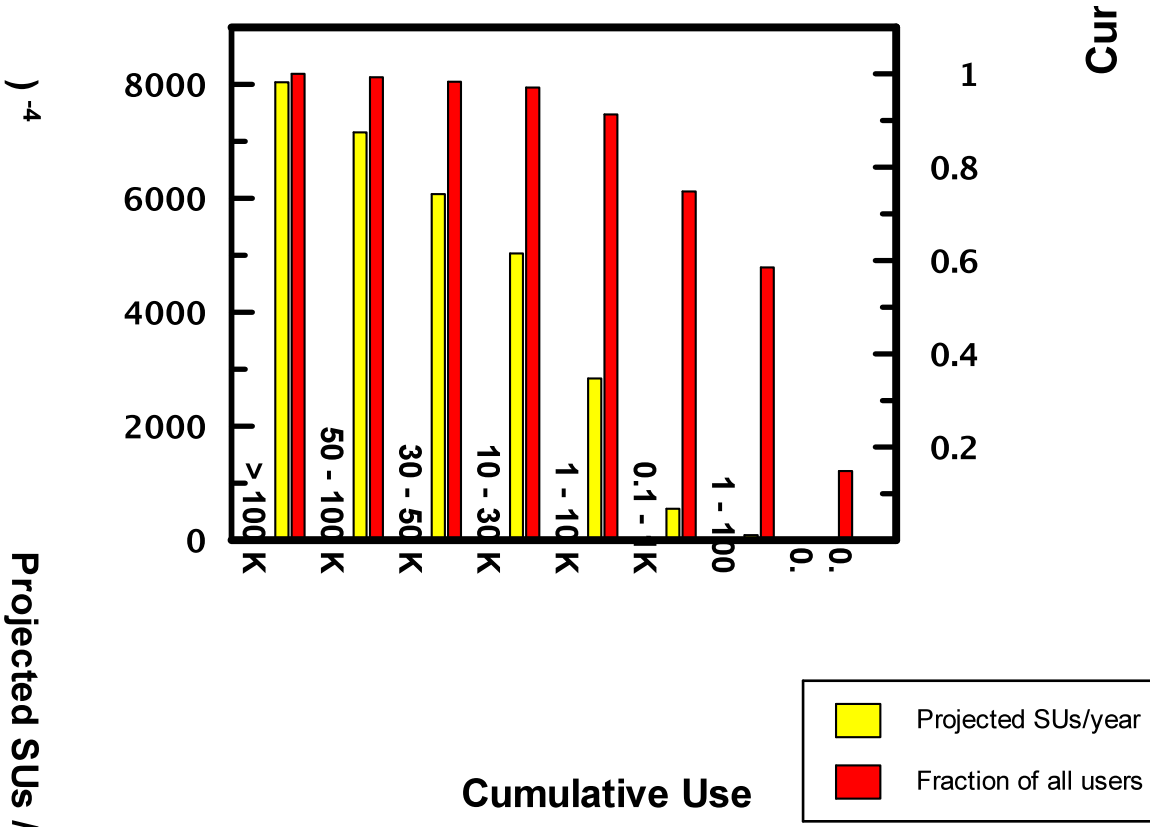
How much growth can we manage?



Establish a Fair Use Policy

- How many SUs should each user be permitted?
- How much influence should affiliation with a US institution have on resource allocation?

Establish a Fair Use Policy



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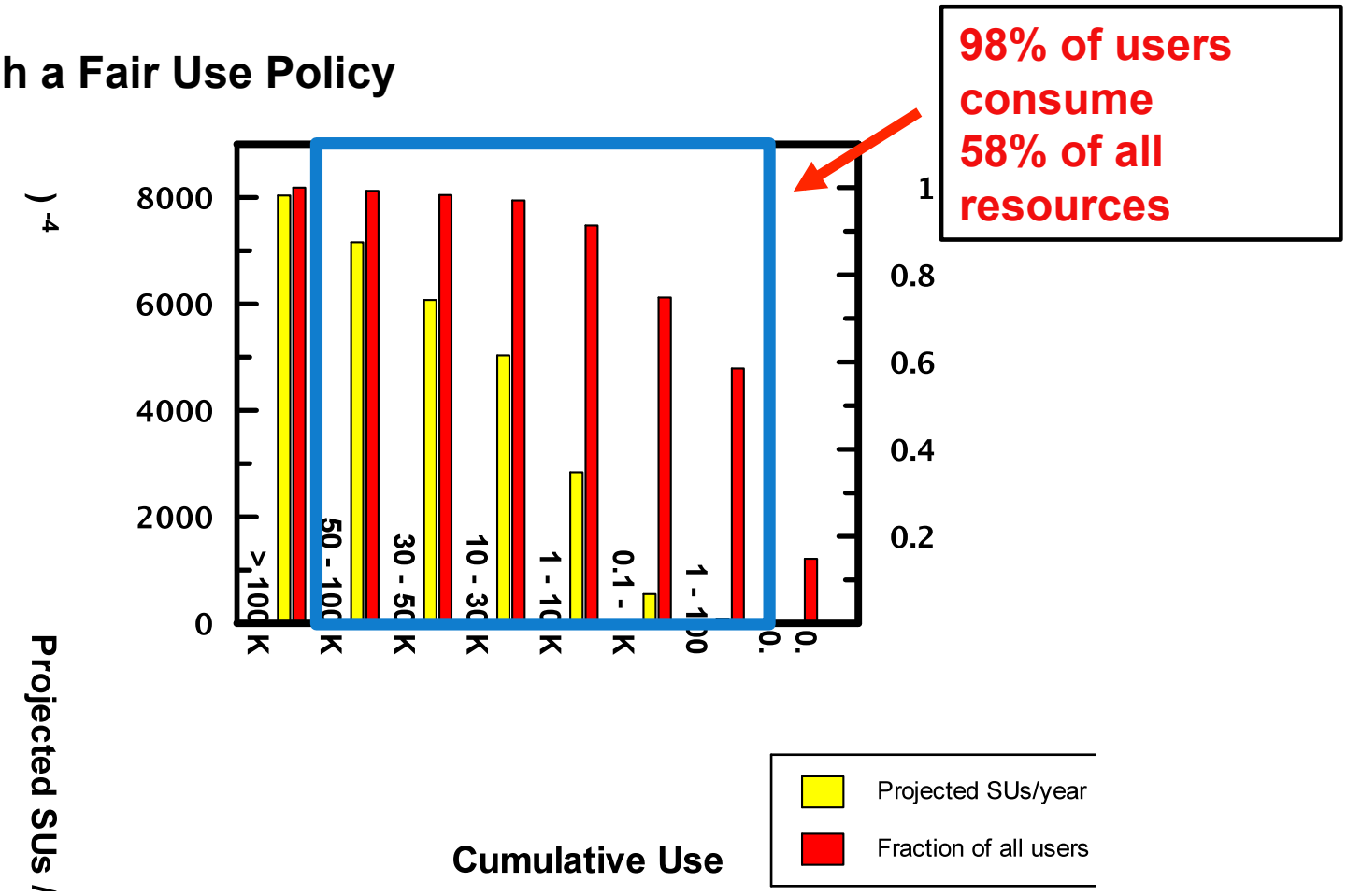

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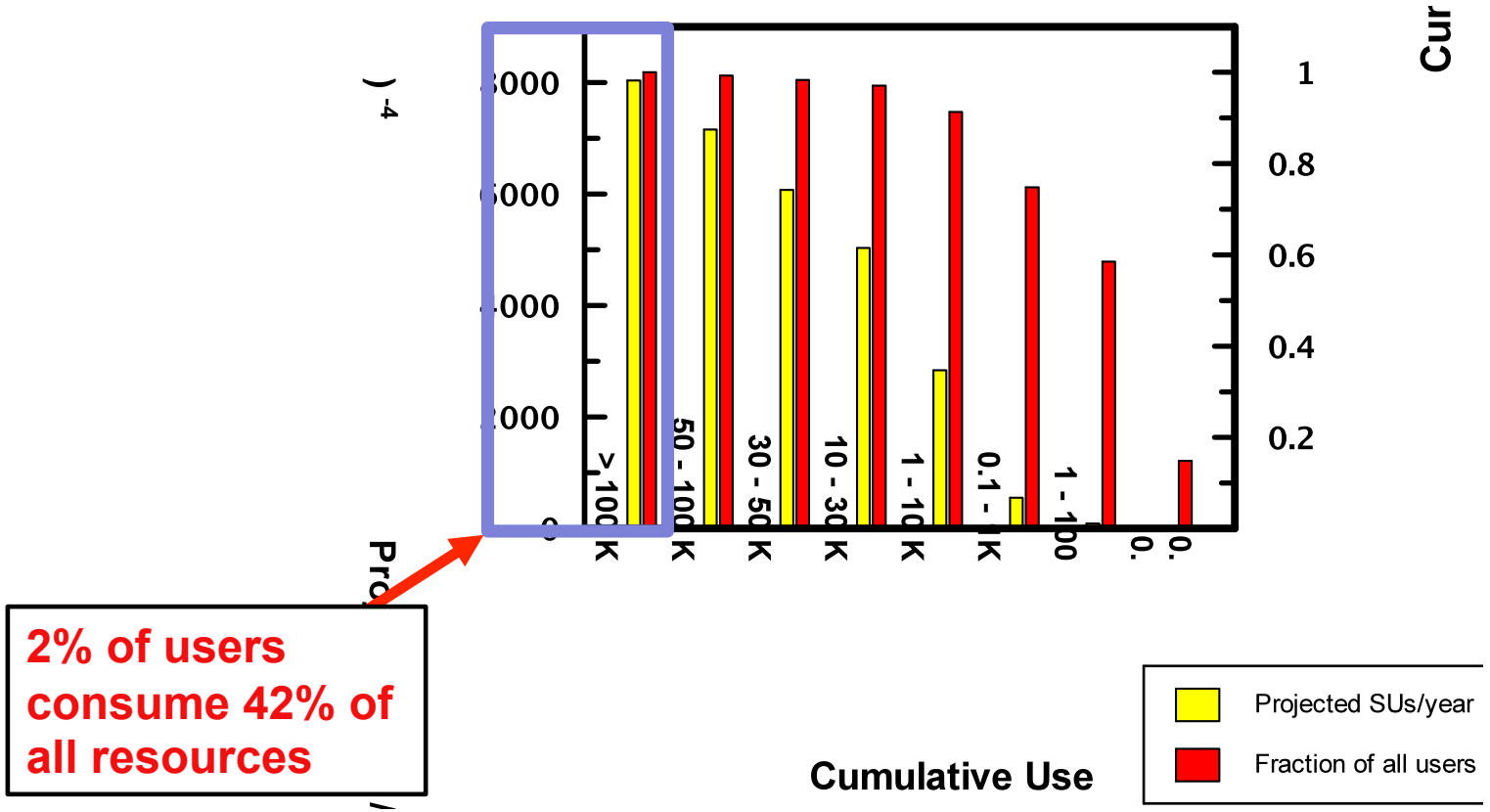

2% of users consume 42% of all resources

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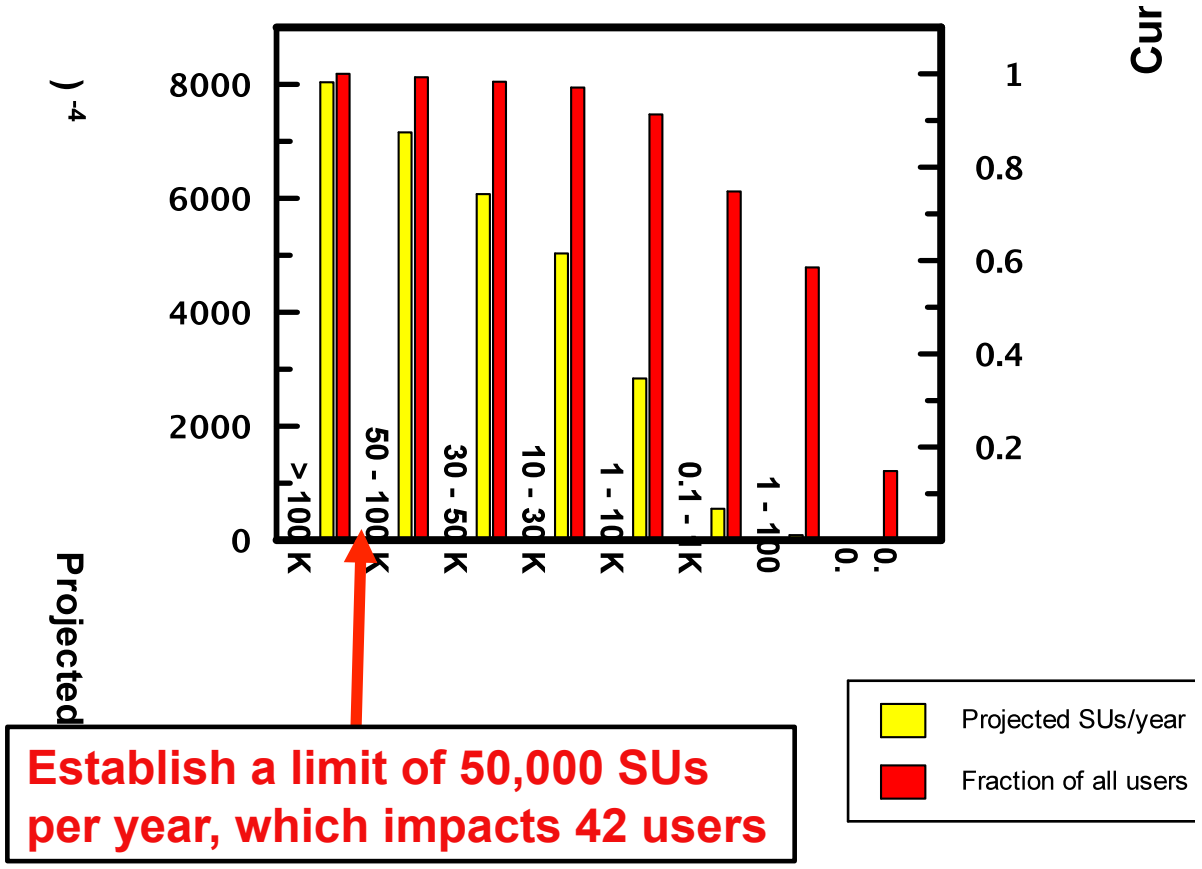


Establish a limit of 50,000 SUs per year, which impacts 42 users

Establish a Fair Use Policy

- Users are permitted to use 50,000 SUs annually from the community allocation. Anyone from any institution can register.
- Users who wish to use in excess of this amount can apply for a personal allocation. This would include users at US institutions and those who have collaborators at a US institution. User can access their allocation using the CSG.

Tools required to implement the CIPRES SG Fair Use Policy:

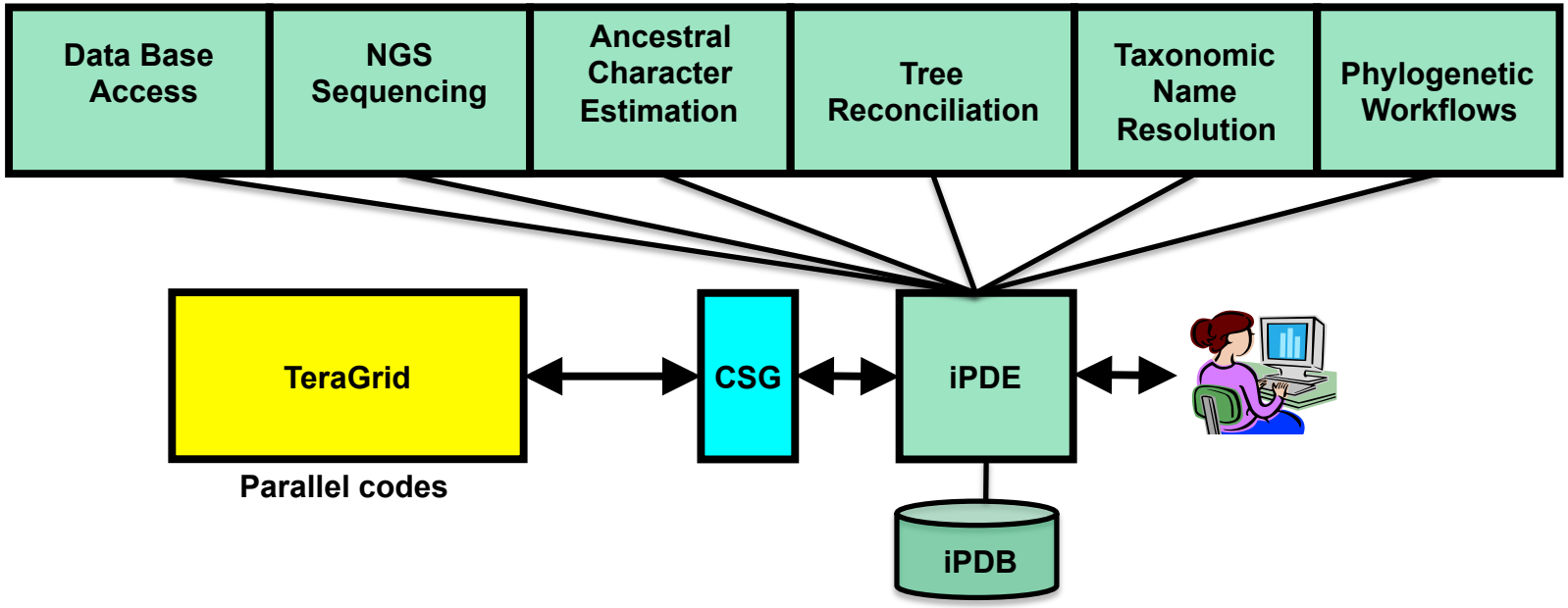
- ability to monitor usage by each account automatically (complete)
- ability to halt submissions from a given user account (complete)
- ability to charge to a user's personal allocation (complete)
- ability for users to track their SU consumption (complete)
- ability to forecast SU cost of a job for users (in progress)

Next Steps:

- Deploy the new user management tools in production.
- Implement the new Fair Usage Policy.
- Add new codes: BEAST, RAxML Light, BEST.
- Partner with the iPlant Project as a service provider.

Next Steps:

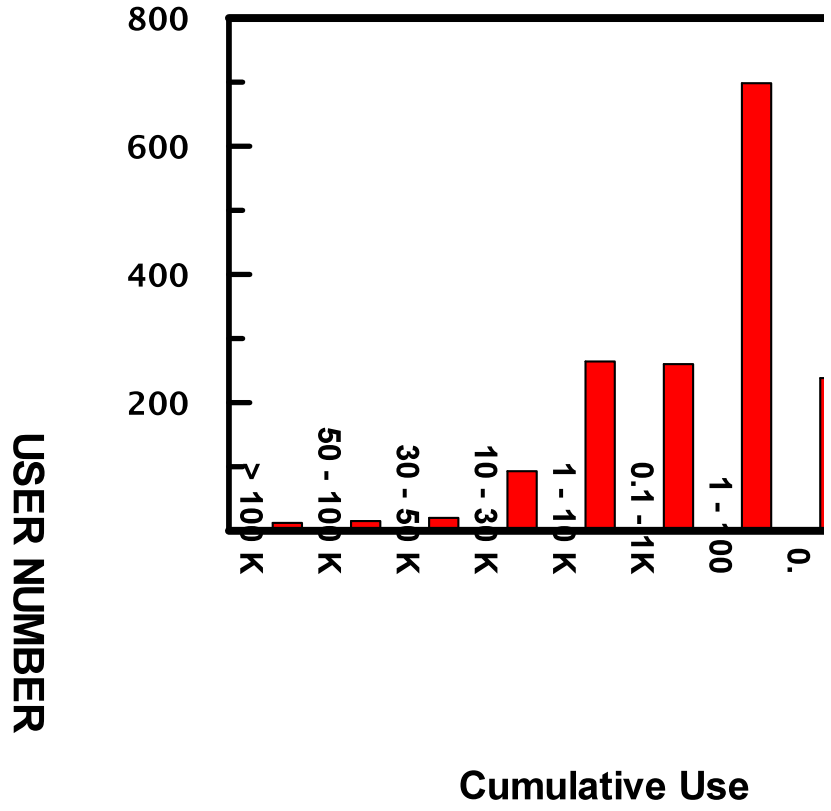
iPlant Collaborative



Acknowledgements:

CIPRES Science Gateway	Terri Schwartz
TeraGrid Hybrid Code Development	Wayne Pfeiffer Alexandros Stamatakis
TeraGrid Implementation Support	Nancy Wilkins-Diehr Doru Marcusiu Leo Carson
Workbench Framework:	Paul Hoover Lucie Chan

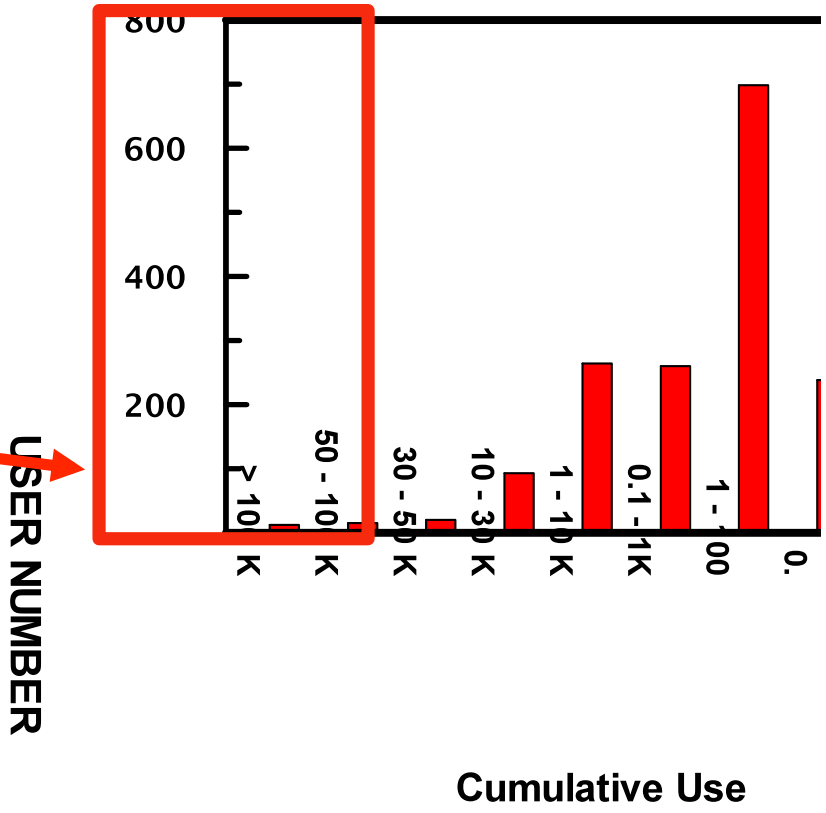
Make sure resource use delivers impact: analyze resource consumption



* Reporting Period: Sept, 2010 – May, 2011

Make sure resource use delivers impact: analyze resource consumption

Who are these users?



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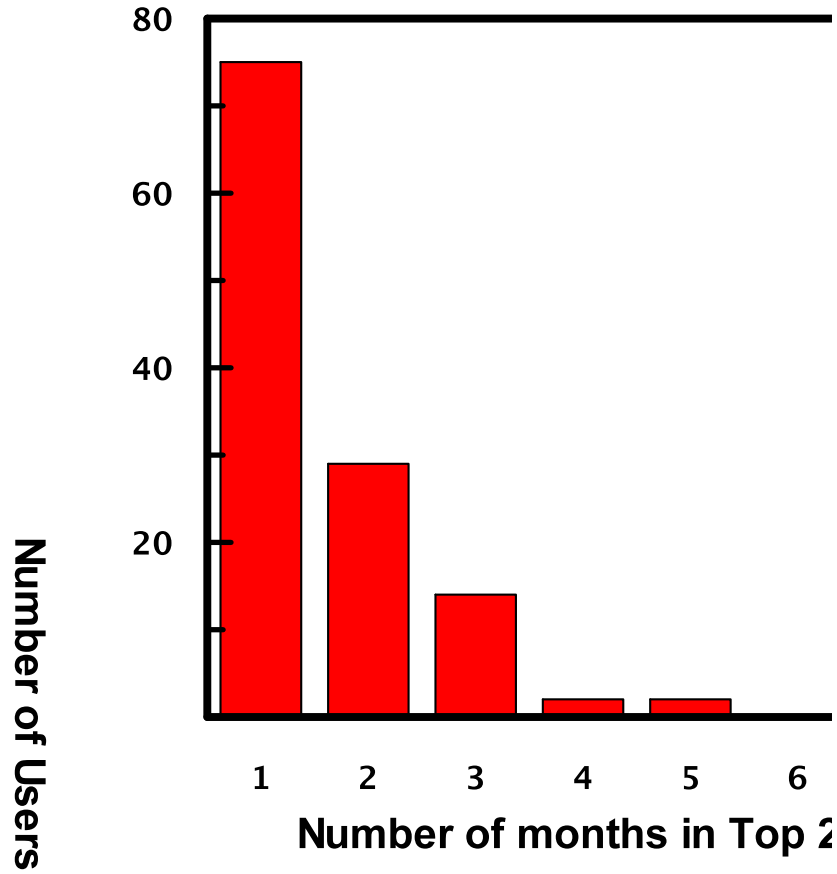
Identify the TOP 20 Users in each month.



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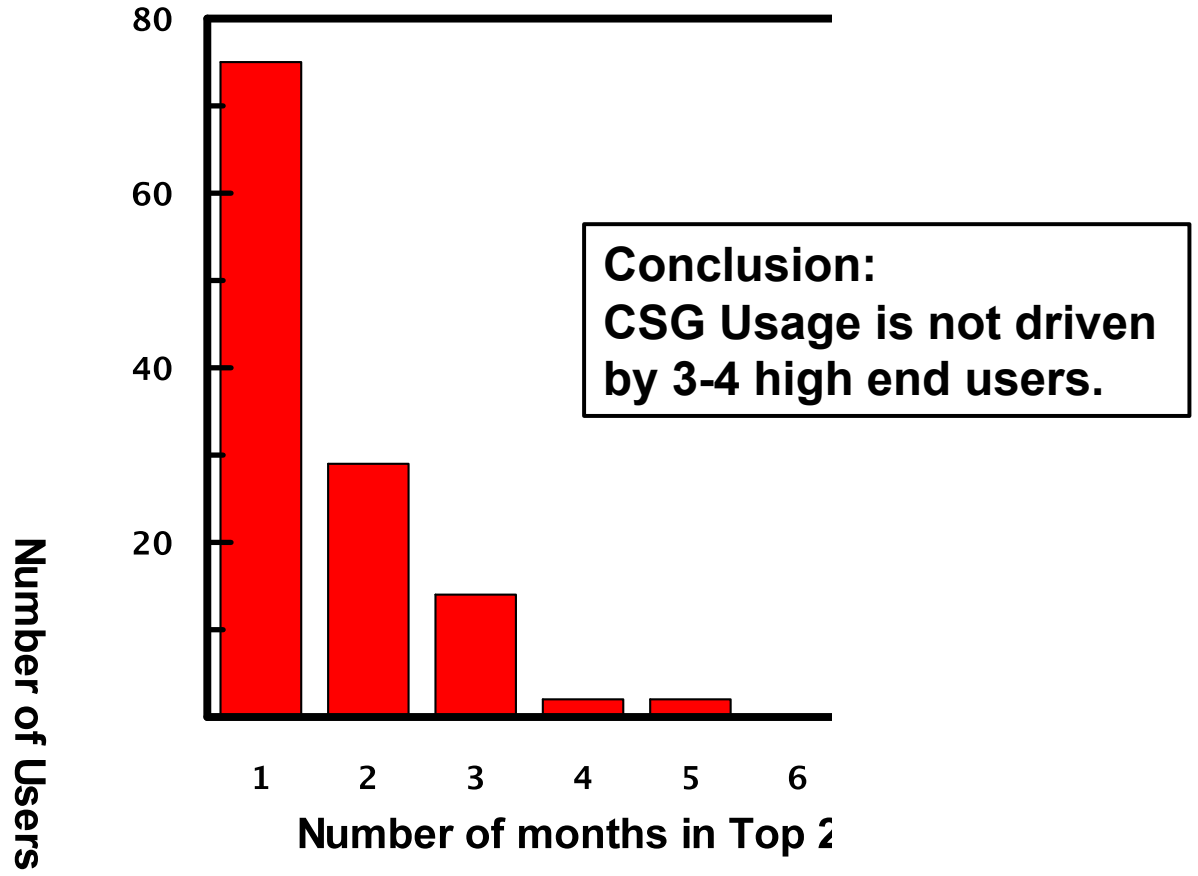

Conclusion:
CSG Usage is not driven by 3-4 high end users.

* Reporting Period: Sept, 2010 – May, 2011

Make sure resource use delivers impact: analyze resource consumption

SUs	% of Users	% total SU
0 – 30 K	97	45
30 – 300,000 K	3	55
> 300,000 K	0	0

* Reporting Period: Sept, 2010 – May, 2011

Make sure resource use delivers impact: analyze resource consumption

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50% of users in this bin are from institutions outside the US

* Reporting Period: Sept, 2010 – May, 2011

Make sure resource use delivers impact: Establish a Fair Use Policy

SUs	Number of Users	% total SU	% per user
< 100	936 (58.5%)	0.2	0.0003
100 - 999	260 (16.3%)	1.6	0.005
1 – 10 K	264 (16.5%)	16	0.06
10 – 30 K	93 (5.8%)	27	0.29
30 – 50 K	20 (1.3%)	14	0.69
50 – 100 K	15 (0.9%)	16	1.06
> 100 K	12 (0.8%)	26	2.14

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Establish 50,000 SUs as the limit for usage from the CSG community account. (Same as Trestles startup account).

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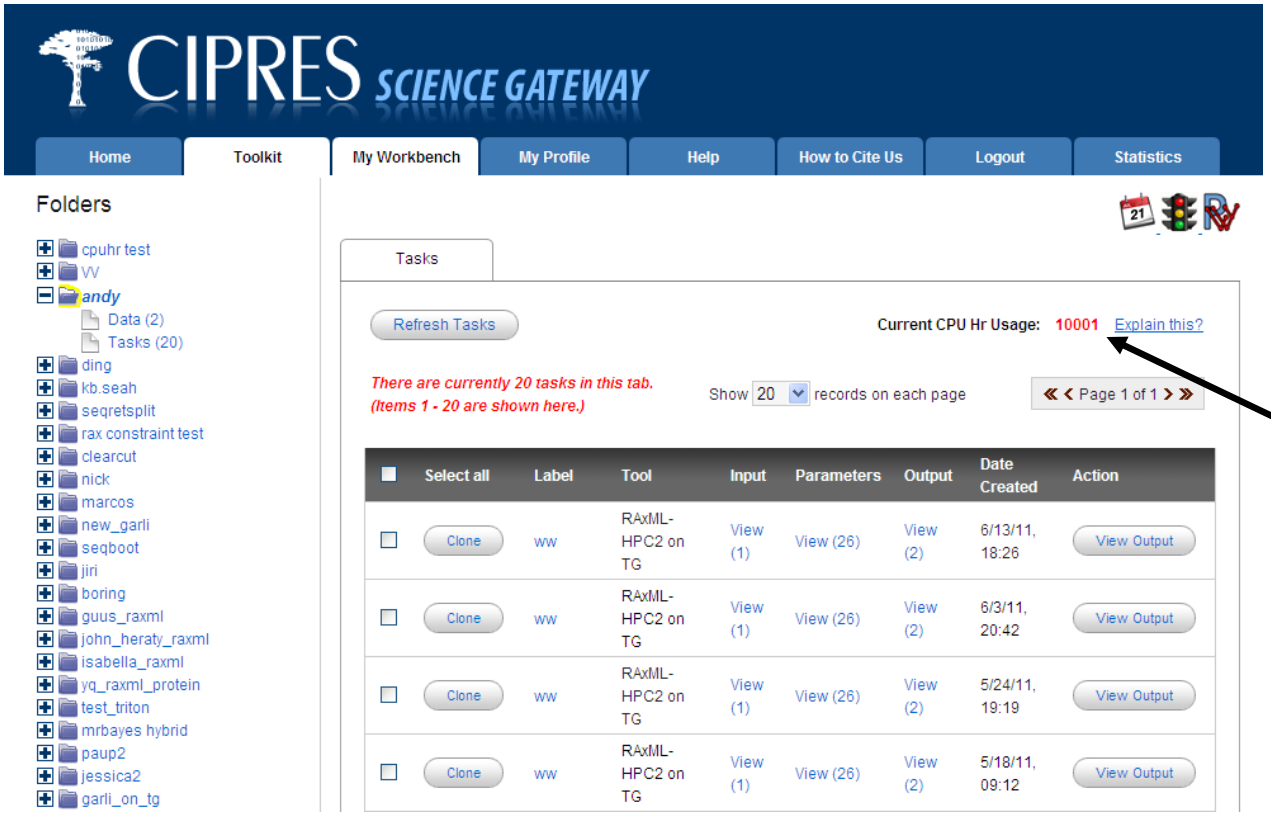
Impacts 42 Users only

Make sure resource use delivers impact: resource consumption



Notify users of their usage level