

BIO\WULF

HIGH PERFORMANCE COMPUTING AT THE NIH

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NIH HPC Staff, CIT

The NIH HPC Core Facility (Biowulf)

- Central scientific compute resource managed by NIH HPC staff (CIT)
- Funded by NIH Capital Investment Fund
- Available to all NIH intramural scientists
- Production facility: high availability, high data durability
- Large scale: 94,000+ processor cores; 25 Petabytes storage capacity
- Enabling research not otherwise possible
- General purpose scientific computing (not dedicated to any one application type)
- 2200+ papers to date based on Biowulf usage



NIH HPC Core Facility

hpc.nih.gov

Biowulf Cluster: High performance computing
For most computational jobs.

Helix: Single shared system: 128 CPUs & 1 TB memory.
Interactive data transfer and file management.

Felix (NIMH only)

Helixweb: web applications (*helixweb.nih.gov*)

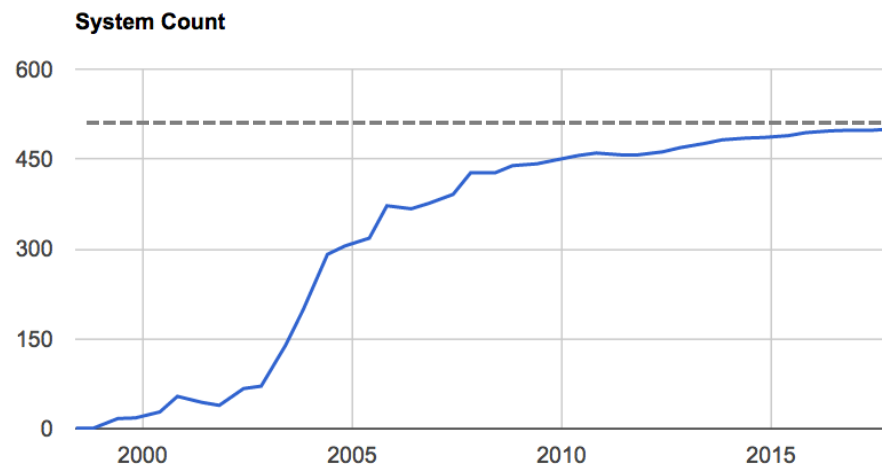
Sciware: run apps on your desktop (e.g. Matlab) (*sciware.nih.gov*)

Biowulf & Helix run the Linux Operating System

RHEL/Centos 7

100% of the Top500 supercomputers run Linux

OPERATING SYSTEM FAMILY / LINUX



List	Count	System Share (%)
Nov 2017	500	100
Jun 2017	498	99.6

Why would you want to use Biowulf?

- Large numbers of jobs (bioinformatics on thousands of sequences)
- Large-memory jobs (whole genome assemblies)
- Parallel jobs with high-cpu demands (e.g., molecular dynamics on 1024 cores)
- Terabytes of data to process
- Multiple or high-performance GPUs

... in other words, LARGE SCALE



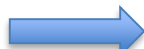
Unsuitable for Biowulf...(or, why bother?)



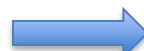
- Small numbers of jobs
- One dependent job after the other
- Interactive jobs, graphics etc.

... in other words, desktops can be pretty powerful!

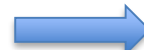
<http://hpc.nih.gov>



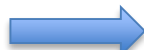
<http://hpc.nih.gov/apps>



User Guides




Announcements



HPC @ NIH

High-Performance Computing at the NIH

[Status](#) [Applications](#) [Storage](#) [User Guides](#) [User Dashboard](#) [How To](#) [About](#)




The NIH HPC group plans, manages and supports high-performance computing systems specifically for the intramural NIH community. These systems include [Biowulf](#), a 90,000+ processor Linux cluster; [Helix](#), an interactive system for short jobs; [Sciware](#), a set of applications for desktops, and [Helixweb](#), which provides a number of web-based scientific tools. We provide access to a wide range of computational applications for genomics, molecular and structural biology, mathematical and graphical analysis, image analysis, and other scientific fields.

Quick Links

- [System Status](#)
- [How To...](#)
- [Application/DB updates](#)
- [User Guides](#)
- [SquirrelMail](#)
- [Policies](#)
- [Training](#)
- [Contact Us](#)

Biowulf Utilization

Monday, December 4th, 2017



Last 24 hrs

71,121 jobs submitted	21 NIH Institutes
43,388 jobs completed	137 Principal Investigators
1,516,083 CPU hrs used	233 users

Announcements


(All)

- **SCHEDULE UPDATE:** Discontinuing SSH to Helix from Outside the NIH Network AND Helix Email to be Retired (Nov 29th 2017)
- **Reminder:** Python in HPC seminar Thursday Nov 30 (Nov 29th 2017)
- **Upcoming Biowulf classes** (Nov 27th 2017)
- **REMINDER:** Walk-In Consult with HPC staff Wed 15 Nov (Nov 14th 2017)
- **Walk-In Consult with HPC staff** Wed 15 Nov (Nov 8th 2017)
- **REMINDER:** Seminar today - Effective use of the Biowulf batch system and storage systems (Oct 30th 2017)
- **NIH Biowulf Seminars:** Making Effective use of the cluster (Oct 24th 2017)


Recent Papers that used Biowulf & HPC Resources

(All publications)


[Natural Language Processing for Large-Scale Medical Image Analysis Using Deep Learning](#)
Hoo-Chang Shin, Le Lu, Ronald M. Summers
in Deep Learning for Medical Image Analysis, Elsevier, (p405-421) (2017)


 [Excessive burden of lysosomal storage disorder gene variants in Parkinson's disease](#)
Robak, LA; Jansen, IE; van Rooij, J et al.
Brain, DOI://10.1093/brain/awx285 (2017)

 [Insights into functions of the H channel of cytochrome c oxidase from atomistic molecular dynamics simulations](#)
Sharma, V; Jambrina, PG; Kaukonen, M; Rosta, E; Rich, PR;
Proc. Natl. Acad. Sci. U.S.A., DOI://10.1073/pnas.1708628114 (2017)

 [Conventional and pioneer modes of glucocorticoid receptor interaction with enhancer chromatin in vivo](#)
Johnson, TA; Chereji, RV; Stavreva, DA; Morris, SA; Hager, GL; Clark, DJ;
Nucleic Acids Res., DOI://10.1093/nar/gkx1044 (2017)

[A joint model for multivariate hierarchical semicontinuous data with replications](#)
Kassahun-Yimer, W; Albert, PS; Lipsky, LM; Nansel, TR; Liu, A;
Stat Methods Med Res, DOI://10.1177/0962280217738141 (2017)

 [Phosphorylated Calmodulin Promotes PI3K Activation by Binding to the SH2 Domains](#)
Zhang, M; Jang, H; Gaponenko, V; Nussinov, R;
Biophys. J., DOI://10.1016/j.bpj.2017.09.008 (2017)

 [Prediction of Host-Pathogen Interactions for Helicobacter pylori by Interface Mimicry and Implications to Gastric Cancer](#)
Guven-Maiorov, E; Tsai, CJ; Ma, B; Nussinov, R;
J. Mol. Biol., DOI://10.1016/j.jmb.2017.10.023 (2017)

[Physiological and pathophysiological implications of PGE2 and the PGE2 synthases in the kidney](#)
Wang, J; Liu, M; Zhang, X; Yang, G; Chen, L;
Prostaglandins Other Lipid Mediat., DOI://10.1016/j.prostaglandins.2017.10.006 (2017)

← Social media, RSS

← <http://hpc.nih.gov/research>

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Accounts



No sharing of accounts!

Apply for an account at

https://hpc.nih.gov/nih/accounts/account_request.php

PI approval needed.

\$35/month flat charge – no additional usage fees

Accounts must be renewed each year.

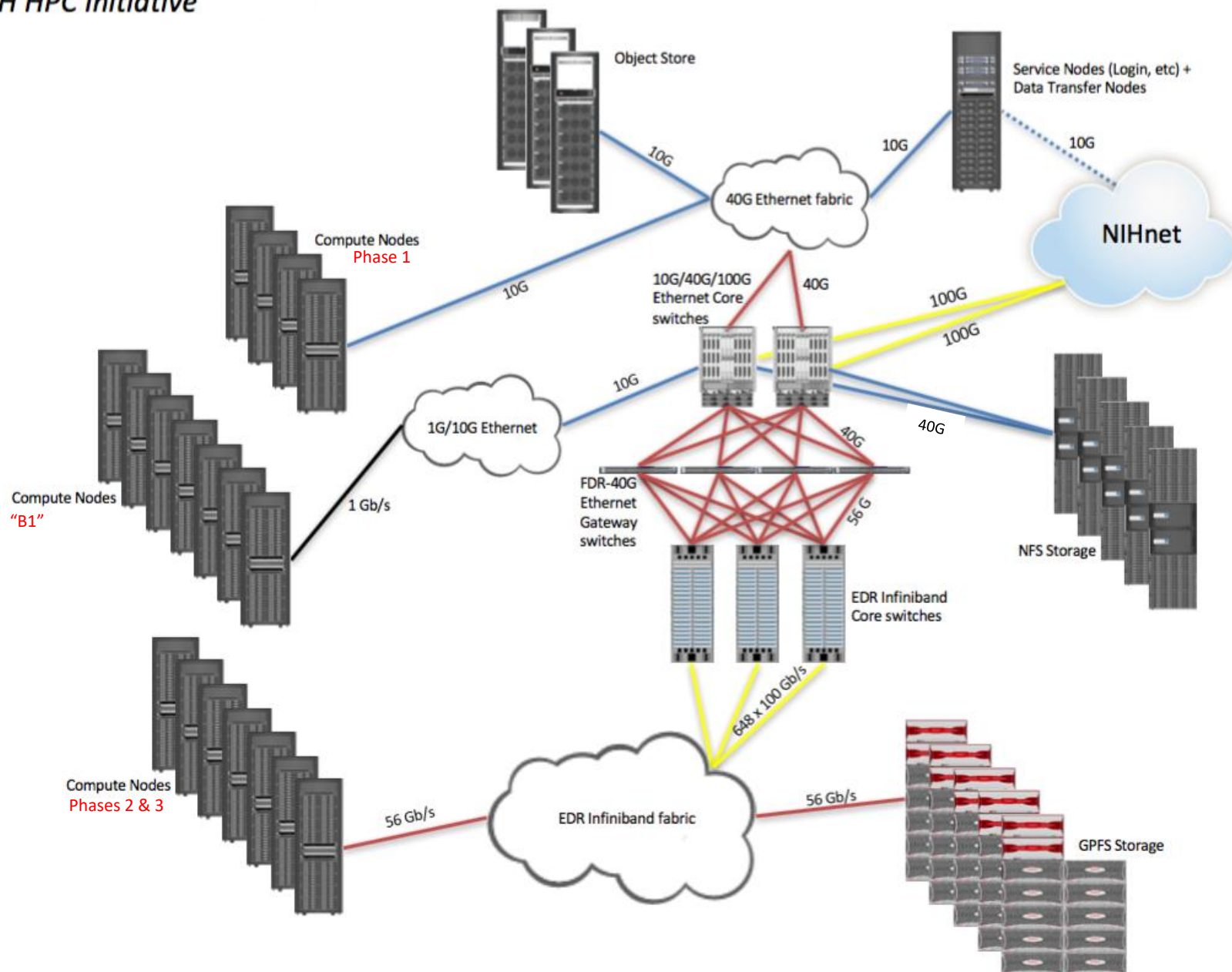
Survey

Linux?

Cluster?

Batch System?

NIH HPC Initiative



Important Concepts

- Computation is performed via jobs that are submitted to the batch queue
- Input data must be transferred to Biowulf filesystems
- Centrally-installed applications are loaded via 'environment modules'
- You can also install/build your own apps in your own Biowulf space

Compute Nodes

# nodes	processor, cores per node	memory	network
1152	Intel E5-2680v4 28 x 2.4 GHz	256 GB	56 Gb/s FDR Infiniband
1080	Intel E5-2695v3 28 x 2.3 GHz	256 GB	56 Gb/s FDR Infiniband
506	Intel E5-2650v2 16 x 2.6 GHz	128 GB	10Gb/s Ethernet
192	Intel E5-2650v2 16 x 2.6 GHz	64 GB	56 Gb/s FDR Infiniband 10Gb/s Ethernet
8	Intel E5-2680v4 28 x 2.4 GHz 4 x nVidia v100	128 GB	56 Gb/s FDR Infiniband
48	Intel E5-2696v4 28 x 2.3 GHz 4 x nVIDIA P100	256 GB	56 Gb/s FDR Infiniband
72	Intel E5-2696v4 28 x 2.3 GHz 2 x nVIDIA K80	256 GB	56 Gb/s FDR Infiniband
24	Intel E5-2650v2 16 x 2.6 GHz 2 x nVIDIA K20x	128 GB	56 Gb/s FDR Infiniband 10Gb/s Ethernet

Buy-In Nodes

# nodes	processor, cores per node	memory	network	funding
72	Intel E5-2680v4 28 x 2.4 GHz	256 GB	56 Gb/s FDR Infiniband	CCR (NCI)
160	Intel E5-2695v3 28 x 2.3 GHz	256 GB	56 Gb/s FDR Infiniband	CCR (NCI)
24	Intel E5-2695v3 28 x 2.3 GHz 2 x nVIDIA K80	256 GB	56 Gb/s FDR Infiniband	CCR (NCI)

- Priority given to funding Lab/IC for 3 years
- Available via *quick* queue to all NIH users

Use of Biowulf's login node

- Submitting jobs
- Editing/compiling code
- File management
- File transfer
- **Brief** testing of code or debugging (under 10 minutes cpu time, < 4 GB memory)





Do not run compute jobs of any kind on the login node!

root

To: [REDACTED]@biowulf2.nih.gov

No compute intensive processes on Biowulf login node

Compute or large memory jobs are not allowed on the Biowulf login node. Such jobs can hang the login node and/or seriously affect all users. If you persist in running such jobs, your account will be locked.

Please use batch or allocate an interactive node if needed. Here is how easy it is to get a dedicated interactive session:

% sinteractive

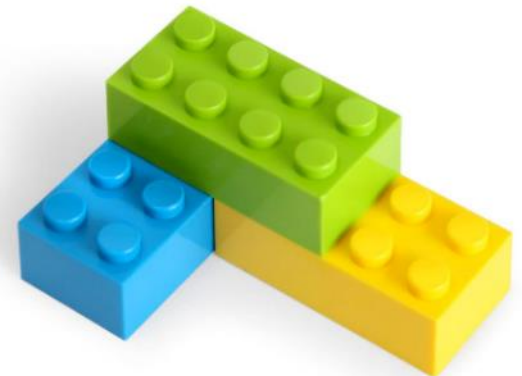
Process terminated:

PID	USER	NI	VSZ	RSS	S	%CPU	%MEM	TIME	COMMAND
23583	[REDACTED]	0	5973256	5463320	R	96.9	4.4	00:01:44	bedtools sort -i KZ946_CLP.bed



Environment Modules

- Dynamically set up environments (paths, library locations, etc.) for different applications
- One easy command for setup (not shell-dependent)
- <https://hpc.nih.gov/apps/modules.html>



How to check quota and usage

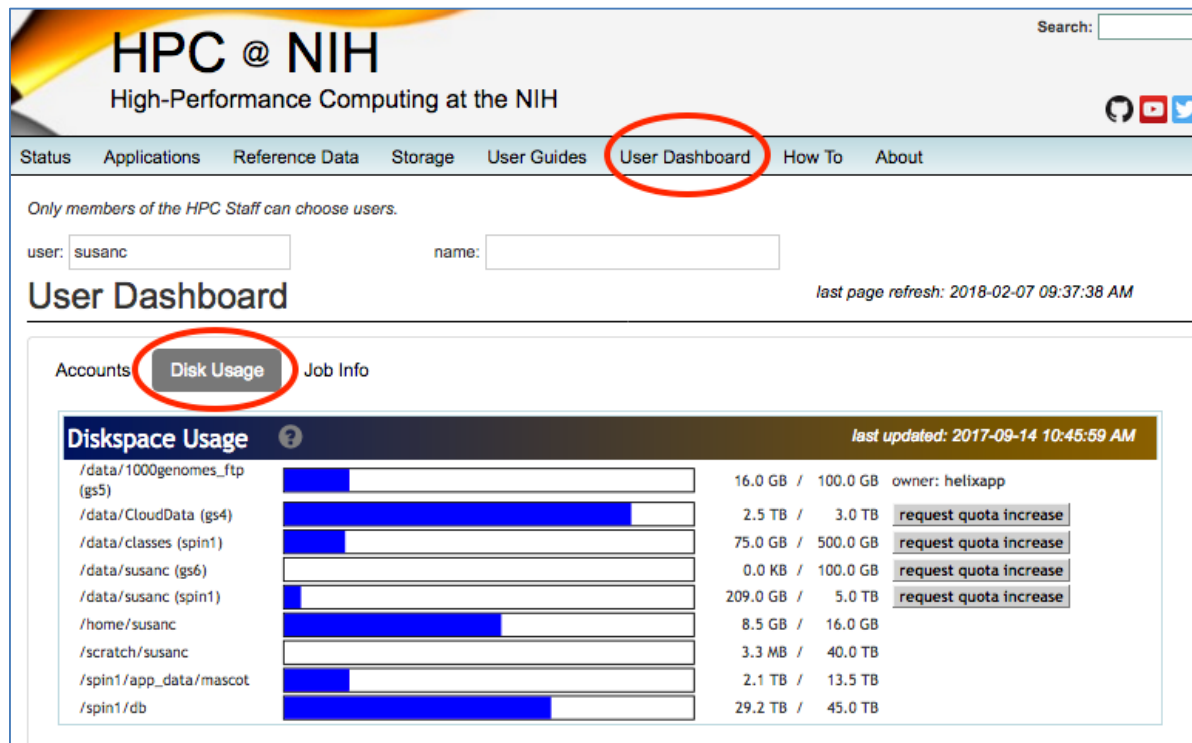
\$ **checkquota**

Mount	Used	Quota	Percent	Files	Limit
/data:	125.8 GB	500.0 GB	25.16%	16529	31129581
/home:	2.4 GB	8.0 GB	30.37%	52888	n/a
ObjectStore Vaults					
teacher:	44.4 GB	465.7 GB	9.00%	n/a	n/a

Quotas and shared directories

- Quota increases for /data
- Shared data directory requests

<https://hpc.nih.gov/dashboard> -> 'disk usage' tab



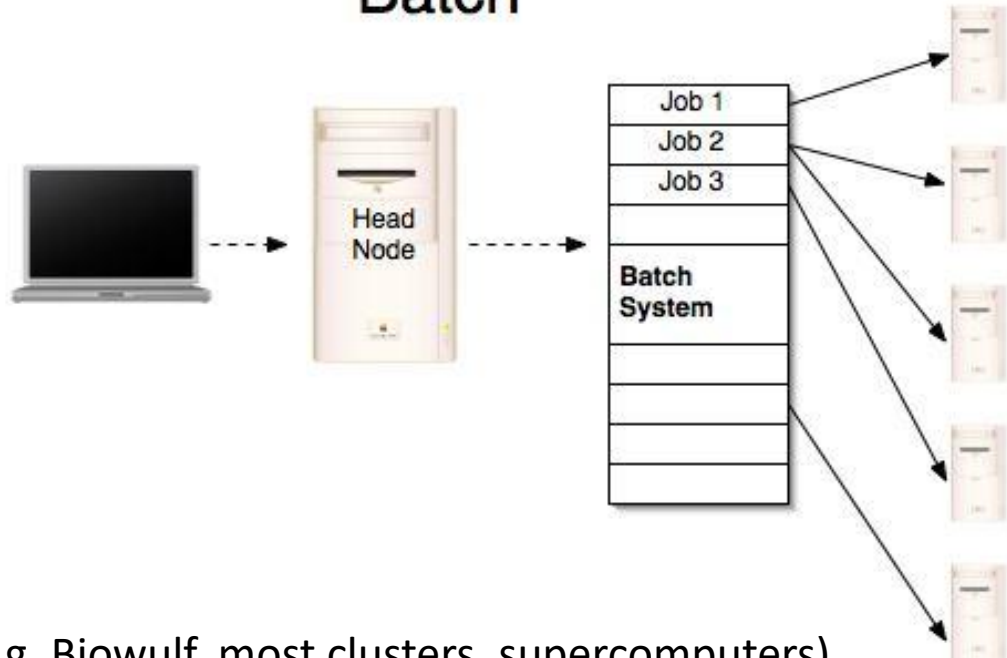
Concepts : Interactive vs. Batch

Interactive

(e.g. your desktop or Helix)



Batch



(e.g. Biowulf, most clusters, supercomputers)



Allocating GPUs

```
sbatch --partition=gpu --gres=gpu:k80:1 jobscript
```

```
sbatch --partition=gpu --gres=gpu:k80:2 jobscript
```

Resource Name	Resource Type	Count Required even if 1
	• k20x	(Max of 2 K20x
	• k80	4 K80
	• p100	4 P100)
	• v100	

(for student accounts, replace --partition=gpu with --partition=student)

Containers

- Biowulf supports Singularity
- Singularity supports Docker containers
- In most cases, build your own container or download from Singularityhub or Dockerhub.
- Containers require root access, and therefore cannot be built on Biowulf

Monitoring Batch Jobs



- Do I have enough disk space for these jobs?
- Core (CPU) utilization?
- Memory utilization?
- Walltime?

Users (you) are responsible for monitoring their jobs



Monitoring Batch Jobs

Command-line Tools for monitoring

- * `squeue`
- * `jobload`
- * `jobhist`

Graphical tool: the HPC dashboard

<https://hpc.nih.gov/dashboard>

Useful URLs

- Biowulf website: hpc.nih.gov
- Biowulf Online Class: hpc.nih.gov/training/intro_biowulf/
- Biowulf User Guide: hpc.nih.gov/docs/userguide.html
- Centrally-installed applications hpc.nih.gov/apps/
- Deep Learning Tools
hpc.nih.gov/docs/deep_learning.html
- Singularity containers: hpc.nih.gov/apps/singularity.html

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Jean Mao



Susan Chacko



Patsy Jones



Jesse Becker



Michael Harris
(intern)



Tim Miller



Afif Elghraoui



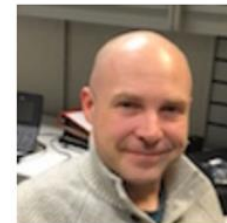
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Antonio Ulloa



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