

Power plus Open OnDemand: facilitating the transition from new to Power user

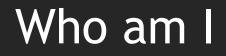
Robert Settlage Advanced Research Computing @Virginia Tech Oct 2020

Ohio Supercomputer Center



It's (almost) that time of year...





- Researcher
- Collaborator
- Educator
- Nvidia DLI Ambassador (CUDA, CV)
- Chemist (PhD, University of Virginia)
- Statistician (MS, Virginia Tech)
- Computational Scientist
- UVA fan



RGINIA



We are Virginia Tech

College Search College Rankings Grad School Search Scholarships \$2,000 No Essay Scholarship 2020 BEST COLLEGES (N)2020 Best College Food in America The 2020 Best College Food ranking is based on meal plan costs and student reviews. Top-NICHE f У ranked colleges offer outstanding on-campus dining-students can easily access heal More 1,382 results Best College Food Best Colleges Best Value *** View On Map #1 Best College Food in America COLLEGE TYPE University of California - Los Angeles 4-Year 4 Year • Los Angeles, CA • 古古古古台 4.977 reviews Private Junior: Campus couldn't be more beautiful. Many spots to study, relax, enjoy the sights, etc. Dorms are pretty standard. Fairly easy to transfer Read 4,977 Reviews Public A+ Overall Niche Grade • A+ Campus Food • Acceptance Rate 16% 2-Year Net Price \$14.760 • SAT Range 1220-1450 Community Will You Get In? Add to List Trade/Career Other #2 Best College Food in America GENERAL AREA OF STUDY 🖗 Virginia Tech 📀 4 Year · Blacksburg, VA · ★★★★☆ 3,752 reviews Any \sim Freshman: As a freshman, I haven't fully experienced Virginia Tech yet, but I can tell that the campus is beautiful, it's a relatively safe school, Read 3,752 Reviews SPECIFIC MAJOR @ A+ Overall Niche Grade • A+ Campus Food • Acceptance Rate 70% Net Price \$18,700 + SAT Range 1180-1360 See All Majors > Will You Get In? Add to List

And well fed

The only school to:

 \checkmark

Sequence and assemble the genome/transcriptome of our mascot

Serve our mascot on Saturdays

 And save said mascot in November



Symposium

Applying Next-Generation Sequencing to Solve Poultry Problems

Next-generation sequencing strategies for characterizing the turkey genome ¹

Rami A. Dalloul ^{*} [∧] [⊠], Aleksey V. Zimin [†], Robert E. Settlage [‡], Sungwon Kim ^{*}, Kent M. Reed

https://doi.org/10.3382/ps.2013-03560

Get rights and content

Presidential Turkeys return to roost at Virginia Tech

For the fourth year, the turkeys will travel from the White House to Gobblers Rest. Meet th newest Hokies at a Dec. 1 open house. Nowmber 22.2019





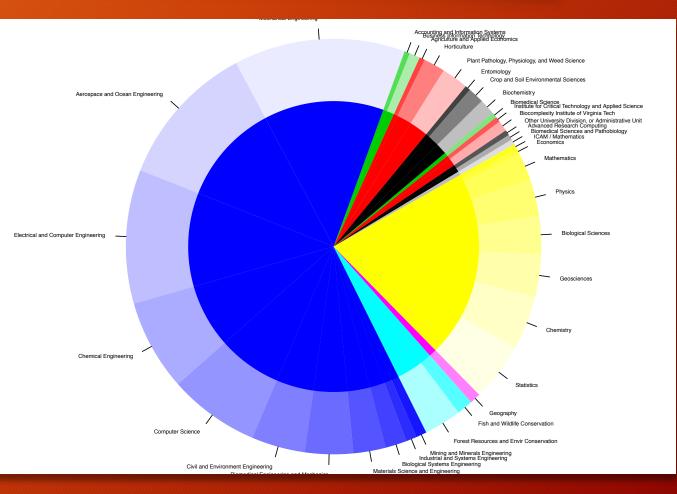


- VT Advanced Research Computing
- The User Spectrum
- Enabling Users with Open OnDemand
- Extending OnDemand to Power
- Providing Feedback on Performance to Improve Resource Utilization (WIP)



VT-Advanced Research Computing (ARC)

- Unit within the Office of the Vice
 President of Information Technology
- Provide centralized resources for:
 - Research computing
 - Visualization
- Staff to assist users
- Website: http://www.arc.vt.edu





ARC - what we do

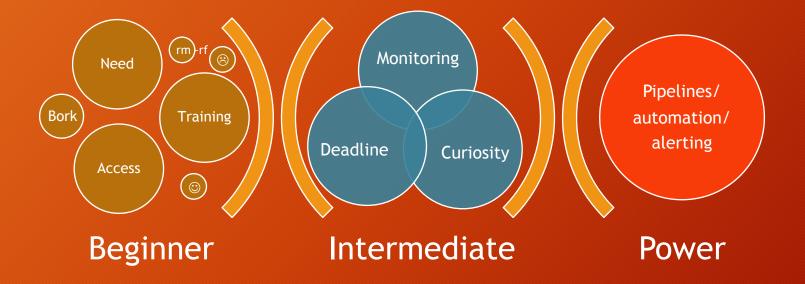
- Advance the use of computing and visualization in VT research
- Centralize resource acquisition, maintenance, and support for research community
- Provide support to facilitate usage of resources and minimize barriers to entry
- Enable and participate in research collaborations between departments
- Provide resources for instruction



Student = user (research powerhouse)

 Odd form of life that tries random stuff to meet random goals while accidently learning

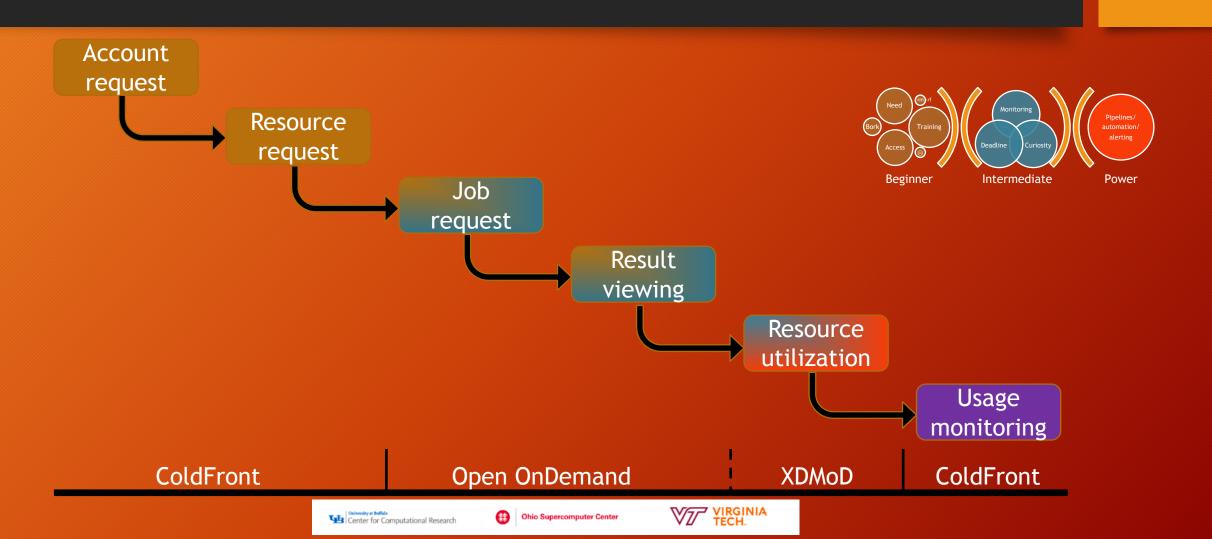
User spectrum







GOAL: Facilitate and speed the progression





🖁 Archive Proje

Getting started on ARC

University at Roffalo

Genter for Computational Research

What do you need?

- An account
- An allocation

| GINIA Advanced Re | esearch Computing | | |
|---|--|------------------------------------|-----------|
| of Information Technology | | | ٩ |
| USER DA | SHBOARD USER INFO V RESOURCES V NEWS V | ABOUT V SUBMIT A REQUEST V | |
| 0. January 2010 | | ACCOUNT | |
| Advanced Research Computing | | HELP | |
| Intel Kanado Anance F Hanard Computing | | CONSULTATION | |
| VIPERINA VIECH | | RESERVE VISUALIZATION RESOURCES | • |
| ARC NEWS | ARC NEWS | ARC NEWS | |
| WHAT CAN ARC DO FOR YOU? | NEW ARC CLUSTER : HUCKLEBERRY | GAS-SURFACE INTERAC | TIONS ARE |

ARC.vt.edu

- Requests
- account request

Coldfront.arc.vt.edu

1. Create a project

B Ohio Supercomputer Center

2. Create an allocation

| | | /////////////////////////////////////// | /////////////////////////////////////// | |
|--|----------------------------------|---|---|--------------|
| https://coldfront.arc.vt.edu | | | 80% | ⊠ ☆ |
| ColdFront - Resource Allo | cation System | | | |
| Home Center Summary Project - Director - Hel | | | | 💄 rsettlag 👻 |
| | | | | |
| Projects » | Allocations » | | | |
| Systems Biology 3036 Teaching | Project | Name | Resource | Status |
| STAT3615 Spring 2020 | Systems Biology 3036 Teaching | SYSB3036 | Compute (Cluster) | Active |
| /groups/hojiang_lab/ | STAT3615 Spring 2020 | lrjohn-STAT3615- | Compute | Andrea |
| /groups/inyoungk_lab/ | | sp20 | (Cluster) | Active |
| /groups/arcsingularity/ | Bovine DNA methylation | bDNA | Compute (Cluster) | Active |
| | | | | _ |
| | ARC-training | arc-train4 | Compute (Cluster) | Active |
| | root | root | Compute (Cluster) | Active |

Open OnDemand 2.0

💄 Add Users 💷 Add Publication 🍷 Add Grant 📝 Update Project Information

| nvestigator: Robert Settlage | (rsettlag) 🖂 |
|------------------------------|--------------|

Description: Open OnDemand setup and configuration

Field of Science: Advanced Research Computing

Project Status: Active

Created: Sep. 04, 2019

Principal I

| 🚢 Users 🗗 | 1 | | 🖾 Er | mail Project | Users 2+ Add Users 2* I | Remove Users |
|-----------|-----------------------|------------------|---------|--------------|-------------------------|--------------|
| Username | Name | Email | Role 🚯 | Status | Enable Notifications () | Actions |
| bbooker | Brandon Booker | bbooker@vt.edu | User | Active | | ئ |
| brownm12 | Matthew Brown | brownm12@vt.edu | User | Active | | 2/ |
| bsawyers | Brandon Sawyers | bsawyers@vt.edu | User | Active | | 2/ |
| efranz | Suppressed Suppressed | efranz@osc.edu | User | Active | | 2/ |
| jdstrick | Justin Strickland | jdstrick@vt.edu | User | Active | | 2/ |
| jkrometi | Justin Krometis | jkrometis@vt.edu | User | Active | | ۵. |
| rsettlag | Robert Settlage | rsettlag@vt.edu | Manager | Active | V | 2/ |

| Allocations 🛾 | | | | + Request Resou | rce Allocation |
|---------------|---------------|-------------------------------|--------|-----------------|----------------|
| Resource Name | Resource Type | Information | Status | End Date | Actions |
| Compute | Cluster | slurm_account_name: ondemand2 | Active | May. 22, 2020 | |



Enabling Users with Open OnDemand

IDGINIA TECH

OSC OnDemand Files -Jobs - Clusters - Interactive Apps -



Ohio Supercomputer Center

An **OH**·**TECH** Consortium Member

OnDemand provides an integrated, single access point for all of your HPC resources.

Message of the Day

2020-03-16 - OSC support during COVID-19 crisis

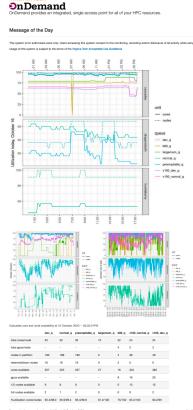
The Ohio Supercomputer Center serves as a critical resource for the public good and, as such, is striving to provide extraordinary support in light of the ongoing COVID-19 crisis. OSC staff are currently working from home but fully expect clients will see no disruption in our services to support this effort.

Examples of the types of special support OSC can provide include: - Priority, unbilled access to OSC computational and storage resources for COVID-19 research - Flexible billing terms and prices for clients anticipating negative economic impacts - Remote, virtual computing lab resources for classroom instructors and educators - Connections to domain experts in academia and industry

Please don't hesitate to contact OSC at oschelp@osc.edu or (800) 686-6472 for more information on this initiative. Please also distribute this message via any communication channel you to which you might have access so that it can be distributed as widely as possible.

CLASSROOM RESOURCES FOR DISTANCE LEARNING

If your class has lost or limited access to computer labs, the Ohio Supercomputer Center might be able to help by



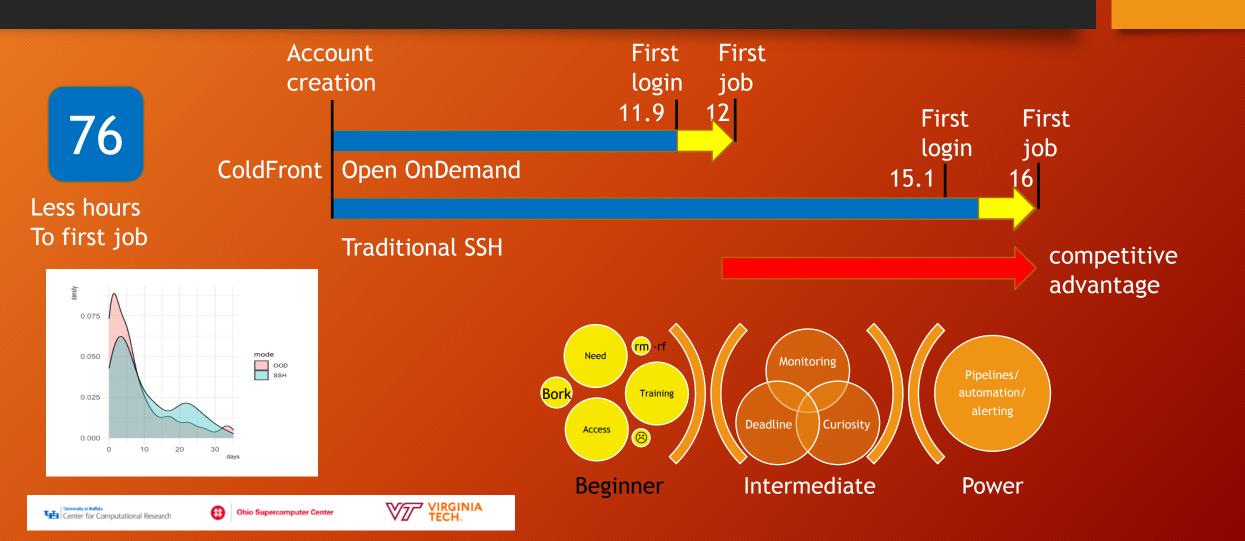
| 530:21PM | | | |
|--------------------------|-----------|-----------|---------------|
| | dev_q | normal_q | preemptable_q |
| total cores/node | 24 | 24 | 24 |
| nodes in partition | 47 | 42 | 47 |
| reserved/down nodes | 0 | 0 | 0 |
| cores available | 209 | 90 | 209 |
| 1/2 nodes available | 8 | 3 | 8 |
| full nodes available | 5 | 1 | 5 |
| Nutilization cores/hodes | 81.5/09.4 | 91.1/97.6 | 81.5/89.4 |

CCR OnDemand Files - Jobs - Clusters - Interactive Apps -NEW USERS: Please run this script in a terminal window (under Clusters menu) before submitting jobs to the cluster. /util/ccr/bin/ssh_no_password.sh MACHINE STATUS: Academic cluster status and Industry cluster status or use 'sostat' command in terminal window NEXT DOWNTIME: Tuesday, October 27, 2020 More details SUMMER SYSTEM UPDATES: We've been busy! Check out all the changes - many directly affect how you run jobs! VIRTUAL WORKSHOPS: Check out our library of virtual workshops More info here FOLLOW US! CCR is now on Twitter! Get system status updates, helpful hints, & highlights of interesting research done at CCR **University at Buffalo** Center for Computational Research OnDemand provides an integrated, single access point for all of your HPC resources. Jobs Efficiency Report - 2020-09-16 XDMoD Z Message of the Day to 2020-10-16 92.3% efficien 7.7% inefficent Welcome to the Center for Computational Research! 1635 inefficent jobs/21184 total jobs You are accessing a University at Buffalo (UB) - Center for Computational Research (CCR) computer system that is provided for CCR-authorized users only. By using this system Core Hours Efficiency Report - 2020-XDMoD Z (which consists of any device attached to this machine, including compute nodes, 09-16 to 2020-10-16 remote visualization software and hardware, storage and database resources), you have implicitly agreed to abide by the highest standards of responsibility to your 42.7% efficient 57.3% inefficent colleagues -- the students, faculty, staff, and external users who share this environment You are required to comply with ALL University at Buffalo policies (http://www.buffalo.edu/ubit/policies/it-policies-a-to-z/computer-and-network-use.html), as well as state and federal laws concerning appropriate use of information technology. 937234.6 inefficent core hours / 1636543.2 total core hours - CCR is not responsible for the loss or misuse of data on our systems CCR systems are NOT HIPAA-compliant. Storage of any personally identifiable Protected Recently Completed Jobs - 2020-09-XDMoD Health Information (PHI) on our systems is a violation of the Health Insurance Portability 16 to 2020-10-16 and Accountability Act (HIPAA) of 1996 Privacy and Security Rules. If in doubt, contact CCR before transferring your data. Date CPU Name - All CCR systems are monitored for administrative and security reasons. Use of this system 4274244 SimRunArray 12 10/5 25.5 constitutes consent to this monitoring for these purposes. 4270864 A slurm s64 10/5 98.5 By continuing to use this system you indicate your awareness of and consent to these terms 4274168 SimRunArray_12 10/5 ind conditions of use. Non-compliance of these terms is considered a breach of University Browser based HPC access

- Zero user install
- Site customizable



Facilitate and speed the progression





Open OnDemand: file management

| VIRGINI/ | ☆ Home Directory ↓ /work/cascades/rsettlag | | | | | | | • un/download |
|-------------|--|-------------------------------|------------------------|--|---|-----------------------------|--------------------------|---|
| D nD | /work/dragonstooth/rsettlag | | File Explorer | | 🖀 Go To >_ Open in Terminal 🔒 New File 🚔 New Dir 🛓 Upload 🗆 | Show Dotfiles | show Owner/Mode | up/download |
| OnDemand | /work/huckleberry/rsettlag | ngle access poin [.] | Home Directory | <pre> /groups/rsettlag_lab/ </pre> | | | | Move/copy/delete |
| OnDernand | /work/newriver/rsettlag | igie access poiri | 🤤 Accelerate_R | | | | _ | mover copyr detete |
| | /groups/ | | 🚘 Escobar_Aug2020 | View C Edit A-z Rename/Move | Download C Copy Paste * (Un)Select All | | 1 Delete | • Edit |
| | | | 🔄 Furong | | | | | Luit |
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| | | | 🚘 Spatial_code | CUDA_testing | | <dir> <dir></dir></dir> | 05/12/2017 09/03/2020 | |
| | | | 🚘 TGICL-2.1 | GPU_testing | | <dir></dir> | 12/20/2017 | |
| | | | 🔄 Wolfram Mathematica | B HOMER | | <dir></dir> | 12/31/2017 | |
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| | | | i 🔁 bin | Novozymes_pipeline Pan_July2018 | | <dir> <dir></dir></dir> | 07/23/2017 07/17/2019 | |
| | | | - Si blueridge | Parkinson_Mar2017 | | <dir></dir> | 03/20/2017 | |
| | | | | Bami_Mar2019 | | <dir></dir> | 03/21/2019 | |
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| | | | - 🔁 easybuild | Valdez_Aug2019 Valdez_May2020 | | <dir> <dir></dir></dir> | 08/26/2019 06/30/2020 | |
| | | | - 🔁 edirect | Valdez_May2020 | | <dir></dir> | 12/31/2017 | |
| | | | 🚘 figure | Valdez_Sept2019 | | <dir></dir> | 06/18/2020 | |
| | | | 🔁 generic_testing_PBS | beegfs_test | | <dir></dir> | 09/03/2019 | |
| | | | 🔄 genomes | 📴 blastdbs | | <dir></dir> | 09/19/2019 | |
| | | | 🚘 glycopat | Class | | <dir></dir> | 09/20/2018 | |
| | | | 🚘 go | | | <dir></dir> | 10/10/2019 | |
| | | | 🚘 gromacs_testing | illumina_vector_contaminants_fasta IaGP | | <dir> <dir></dir></dir> | 06/01/2020 09/07/2019 | |
| | | | 🚘 huckleberry | Solution States | | <dir></dir> | 05/02/2018 | |
| | | | 🚘 intel | i ncbi-blast-2.10.1+ | | <dir></dir> | 09/28/2020 | |
| | | | 🚘 inyoungk | 📴 test_pipeline | | <dir></dir> | 03/01/2019 | |
| | | | 🗀 live_demo | Craig_Oct2016_laptop.tgz | | 354.56mb | 08/30/2019 | |
| | | | 🚘 mapping_test | Davy_July2017_laptop.tgz | | 627.42mb | 08/30/2019 | |
| | | | - 🔄 mass_spec_software | Drvisis_Oct2013.tar Pan_July2018_laptop.tgz | | 187.29gb 698.94mb | 06/14/2016 08/29/2019 | |
| | | | - 🔄 mdahshan_R | Pan_July2018_laptop.tgz | | 36.82mb | 08/29/2019 | |
| | | | - 🔁 mxnet | Valdez_April2019.laptop.tb2 | | 172.75mb | 09/05/2019 | |



| ∀7 7 | OnDemand Files- | Jobs - | Clusters - | Interactive Apps - | 7 | > Develop ~ | | | | | |
|-------------|------------------------|-------------------|-----------------------|--|---|---|---|--|--|--|--|
| | | | >_Dragons | es Shell Access tooth Shell Access erry Shell Access | Acceptable Use | Guidelines (http://www.policies.vt. | edu/acceptable | use.php) + | | | |
| | OnDemand provide | | | | i cocond f | prise Directory Password authenticat actor challenge. After your passwor eive a DUO challenge. | | | | | |
| | | | | | Information systems, plus | Oct 16 18:00:38 2020 from ondemand-p on and examples of how to use huckle s forms for requesting accounts or s available at http://www.arc.vt.edu. | berry and othe berry and othe | | isb-1.opc.v | /t.edu | |
| | | | | | data usage: USER rsettlag | ondemand stat5014-fall20 arctest mabrownlab ondemand2 IGAL2018 ARC-train2 MinION_seq valdez.seq_2 | DATA (G1B) 355.4 318.0 101.0 229236.0 6161.0 4256.0 20219.0 0.0 55.0 171.0 7696.0 5924.0 311.0 27598.0 0.0 5924.0 311.0 27598.0 0.0 920.0 101.0 0.0 CLUSTER all all all all all all all all all al | 000TA (GiB) 640 20480 20480 20480 10240 10 | FILES 495877 147912 32430041 168990 24799 981446 4 204 9 2228 1780 26353 2981335 579 83018 147912 2 LEFT (hrs) Infinity | 0000TA - 6291456 104857600 5242880 5242880 5242880 5242880 5242880 5242880 5242880 5242880 5242880 5242880 10485760 10485 | |

- OOD knows who you are
- Authentication is done via Browser
- SSH window doesn't re-2FA





Open OnDemand: interactive apps

| V InDemand Files Jobs Clusters | Interactive Apps - | Interactive Apps [Sandbox] |
|--|---------------------------------------|-----------------------------|
| | | Cascades |
| | Cascades | MANSYS Workbench |
| VIRGINIA TECH | acis BYO-Container | acis BYO-Container |
| | COMSOL Multiphysics | COMSOL Multiphysics |
| OnDemand | 🥃 Jupyter Notebook | Example Shiny App |
| OnDemand provides an integrated, | si ir | 🥃 Genome Browser |
| | Gi G Jupyter Notebook (Julia-enabled) | 🚔 Jupyter Notebook |
| | Supyter NotebookContainer | 🥃 Jupyter NotebookContainer |
| | 📣 MATLAB | 👌 LaBB-CAT |
| Message of the Day | III ParaView | A MATLAB |
| | | NSIGHT |
| | Remote Desktop | III ParaView |
| This instance of Op | 🗲 🤹 Rstudio 🛛 🕻 | « QGIS |
| What this means is that we use it for testing new fu | - Stata | 🌣 Remote Desktop |
| | VisIT | Remote Desktop |
| For a stable instance of OnDemand, please use: | | 🗢 Rstudio |
| | | stata |
| | | state pymol |

• System wide apps

super_test

• User developed apps



Open OnDemand: interactive apps

| RStudio Server (Owens and Pitzer) (11421197.owens-batch. | ten.osc.edu) | 1 node 1 core R | lunning | |
|--|---|--------------------------|---------------------|-----------------------------|
| Host: >00456.ten.osc.edu Created at: 2020-10-16 18:09:41 EDT | | | Delete | |
| Time Remaining: 1 hour Session ID: d842589d-cc50-41bb-8a87-32b2d62cf49b | MATLAB (11421211. | owens-batch.ten.osc.edu) | | 1 node 1 core Running |
| R Connect to RStudio Server | Host: >00467.ten.osc.edu Created at: 2020-10-16 Time Remaining: 1 hou Session ID: 5d9be97c-0 | 18:11:57 EDT | | Delete |
| Reverse proxy setup automated | noVNC Connection | Native Instructions | | |
| NoVNC Image/connection settings | Compression | 0 | Image Quality | |
| Direct SSH to nodeView only sharable link | 0 (low) to 9 (high) Launch MATLAB | | 0 (low) to 9 (high) | View Only (Share-able Link) |



Open OnDemand: form based jobs

٢

•

BYO-Container

This app will build a **user** Singularity container GUI on the Cascades cluster. The app will exit once the build is complete.

Container to build e.g. docker://alpine:latest

docker://nvcr.io/nvidia/tensorflow:20.06-tf2-py3

- This should be the full container name from the registry
- This will run: singularity pull -- force container
- Creating: /work/cascades/PID/singularity/container_tag.sif

✓ use cache if checked -- COMING SOON

Unchecked adds flag --disable-cache to pull command

Slurm account

2

Choose the partition to run in. This will be an 8 core job.

v100_normal_q

I would like to receive an email when the session starts

Launch

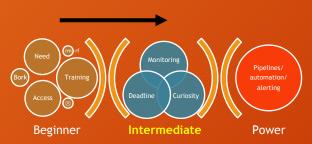
* All BYO-Container session data is generated and stored under the user's home directory in the corresponding data root directory.

- Same mechanism for GUI app launch can drive scriptable jobs
- Further simplify standard workflows
 - parameter sweeps
 - Production codes
 - Monitoring workflows

Open OnDemand: job composer

Support transition from GUI prototyping to scripting (and back for result exploration)

- Job composer brings familiar tools to scripting
- Web based interaction with schedulers
- Web based script editing
- Scripts from templates
- Web based job monitoring



| rototyping to scripting | VT OnDemand / Job Composer | Jobs Templates | | | | 9 Help |
|---|---|---|--------------------------------------|-------------------------------|---|---------------|
| oration) | Job was successfully updated. | | | | | × |
| | Jobs | | | | | |
| | + New Job + | | | オ Create Template | | |
| | (2) Edit Files 🌣 Job Options ≻ Open Terr | ninal Stop | | Telete | Job Details Job Name: | |
| iliar tools to scripting | Show 25 • entries | | Search | | (default) Simple Sequential Python Job Submit to: | |
| iliar tools to scripting | Created IF Name September 17, 2020 10:10am (defa | e Iî ult) Simple Sequential Python Job | ID J1 Cluster | 11 Status 11 Not Submitted | Huckleberry | |
| ith schedulers | | ult) Simple Sequential Job | Cascades | Not Submitted | Account: | |
| | | | 418809 Cascades | Completed | Not specified | |
| | | ult) Simple Sequential Python Job | 418397 Cascades 64053 Huckleberry | Completed | Script location: | |
| | | | 64177 Huckleberry | Completed | /home/rsettlag/ondemand/data/sys/myjobs/projects/default/14 | |
| | May 20, 2019 2:49pm (defa | ult) Simple Sequential Job | 94442 Cascades | Completed | Soript name: | |
| | May 16, 2019 10:39am (defa | ult) Simple Sequential Job | 53507 Huckleberry | Completed | | |
| lg | Showing 1 to 8 of 8 entries | | | Previous 1 Next | Folder Contents: | |
| | | | _ | | /main_job.sh | |
| VT OnDemand / Active Jobs | | | | | | |
| | | Your Jobs - All Clusters - | | | Submit Script | |
| | | | | | main_job.sh | |
| Active Jobs | | | | | Script contents: | |
| Show 50 • entries | | Filter: | | | #:/bin/bash #SBATCHjob-name=python_script #SBATCHtime=01:00:00 | |
| ID Iî Name lî User | l↑ Account l↑ Time Used l↑ Que | ue ⊥î Status ⊥î Cluster ⊥î | | | #SBATCH -n 1 | |
| > 323223 qstat.30 rsettiag | | nal_q,dev_q Quoued Dragonstooth | | | # A Basic Python Serial Job # # The following lines set up the Python environment | |
| 323222 qstat.20 rsettlag 323220 qstat.10 rsettlag | | nal_q,dev_q Queued Dragonstooth | | | module load Anaconda/5.2.0 source activate pearc20 | |
| 323219 qstat.00 rsettiag | | nal_q,dev_q Queued Dragonstooth | | | # # Move to the directory where the job was submitted from # You could also 'cd' directly to your working directory | |
| > 323218 qstat.50 rsettiag | arctest norm | nal_q,dev_q Queued Dragonstooth | | | cd \$SLURM_SUBMIT_DIR # | |
| > 323216 qstat.40 rsettlag | arctest norm | nal_q,dev_q Oucced Dragonstooth | | | # Run Python # python hello.py | |
| Showing 1 to 6 of 6 entries | | Previous 1 Next | | | | C Open Dir |

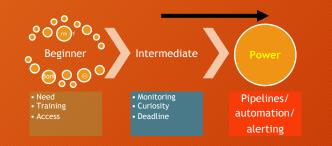


Open OnDemand - XDMoD integration

| Ruby Cluster 🖿 Pitzer Cluster 🖿 Owens Cluster | Ruby Cluster La Pitzer Cluster La Owens Cluster | | | OnDemand Files - Jobs - Clusters - Interactive Apps - 💣 🎬 | | | | |
|--|---|--|--|--|---|--|--|--|
| Ruby Cluster Status 52 of 226 Nodes Active (174 Nodes Pree) 2301% | 368 of 662 Node 55.59% | Cluster Status es Active (294 Nodes Free) | | Chio Supercomputer Center An OH-TECH Consortium Member OnDemand provides an integrated, single access point for all of you | Ir HPC resources | | | |
| 1040 of 4504 Processors Active (3464 Processors Fi 23.09% 0 of 20 GPU Nodes Active (20 Node(s) Free) | 34.73% 74 of 78 GPU No | ors Active (19486 Processors Free) odes Active (4 Node(s) Free) | | Message of the Day | Jobs Efficien Report - 2020 to 2020-10-19 | | | |
| 105 | | 94.87% | | 2020-03-16 - OSC support during COVID-19 crisis | 75.0% efficient | | | |
| 4 Running or Queued Jobs (and 165 blocked jobs) | 647 Runnin | ng or Queued Jobs | | The Ohio Supercomputer Center serves as a critical resource for the public good and, as such, is striving to provide extraordinary support in light of the ongoing COVID-19 crisis. OSC staff are currently working from home but fully expect clients will see no disruption in cur services to support this effort. | 2 ineffice | | | |
| Queued 0 (0 requesting C | | 358 (111 requesting GPU) | | Examples of the types of special support OSC can provide include: - Priority, unbilled access to | | | | |
| | | | | OSC computational and storage resources for COVID-19 research - Flexible billing terms and prices for clients anticipating negative economic impacts - Remote, virtual computing lab resources for classroom instructors and educators - Connections to domain experts in academia | Core Hours Efficiency Re 2020-09-19 to | | | |
| | Owens Cluster Status | | | and industry Please don't hesitate to contact OSC at oschelo@osc.edu or (800) 686-6472 for more information | 98.1% efficient | | | |
| 398 of 813 Nodes Active (415 Nodes Free) 48.95% | | | | on this initiative. Please also distribute this message via any communication channel you to which you might have access so that it can be distributed as widely as possible. | | | | |
| 10171 (| f 23036 Processors Active (12865 Processors Free) | | | CLASSROOM RESOURCES FOR DISTANCE LEARNING | 0.0 inefficen | | | |
| | | | | If your class has lost or limited access to computer labs, the Ohio Supercomputer Center might t able to help by providing no-cost access to cloud computing resources. Classes and workloads | | | | |
| 55 35.48% | i of 155 GPU Nodes Active (100 Node(s) Free) | | | aure to risp or provine is information acceler to used derivating instructives. Classes and worksaks any size can gain access. SSC's web-vorwer infraface to its substantial funct computer system provides novice users with virtual desktops preloaded with applications, such as MATLAB, RStudio, or Jupyter Notebook. | | | | |
| | 287 Running or Queued Jobs (and 21 blocked jobs) | | | As an example, an OSU undergrad statistics class recently used iPads to remotely access RStud on OSC systems. We can provide online demonstrations or evaluations and potentially add | O ID Ne | | | |
| Bunning | 287 | | | additional software packages. | 11421211 on | | | |
| Queued | 0 (0 requesting GPU) | | | Please contact OSCHelpticosc.edu to talk to OSC about distance-learning support options available to you. | 2 /di /sy | | | |

XDMoD provide job level performance data analytics

- Power users search for available hardware features •
- Power users are cognizant of hardware capabilities



mobile device friendly

Jobs Efficiency Report - 2020-09-19 to 2020-10-19

2 inefficient jobs /8 total jobs

0.0 inefficent core hours/2.0 total core bours

Efficiency Report -2020-09-19 to 2020-10-19

cently Completed bs - 2020-09-19 to

/dashboard /sys/bc_osc_mati

75.0% efficient

Open XDMoD

25.0% inefficer

Open XDMoD

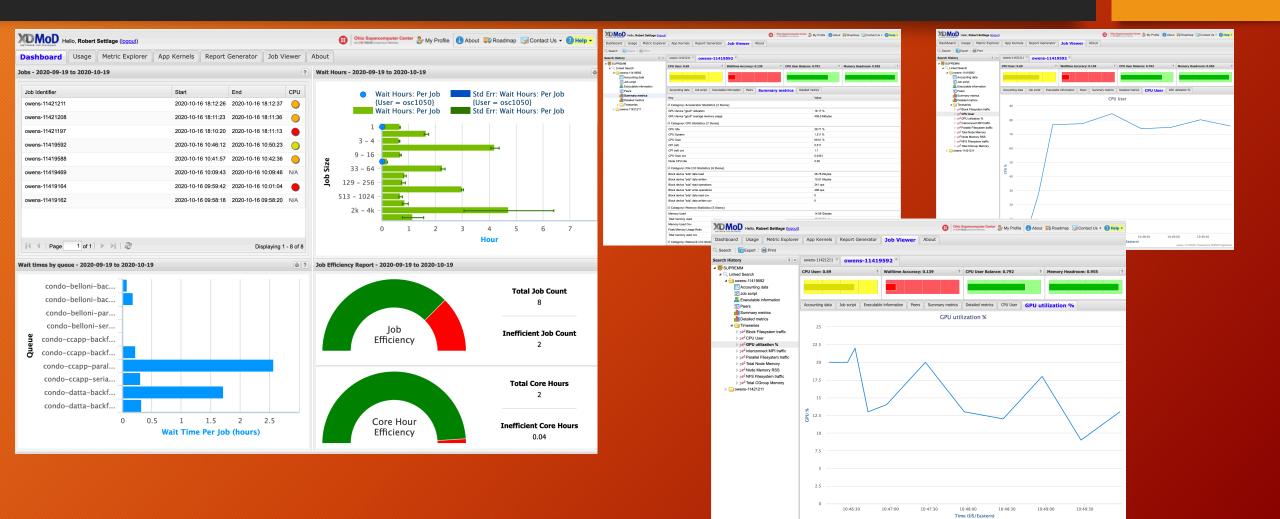
1.9% ineffice

10/6

| Jobs Effic to 2020-1 | tiency Report - 2020- 0-16 | 09-16 XDMoD Z |
|---|--|---|
| 92.3% effi | cient | 7.7% inefficent |
| 16 | 35 inefficent jobs/2118 | 4 total jobs |
| | rs Efficiency Report 2020-10-16 | - 2020-XDMoD 🖊 |
| | | |
| 42.7% effi | | |
| 937234.6 i | nefficent core hours / 16 hours Completed Jobs - 20 | 36543.2 total core |
| 937234.6 i Recently | nefficent core hours / 16 hours Completed Jobs - 20 | 36543.2 total core |
| 937234.6 i Recently 16 to 202 ID | nefficent core hours / 16 hours Completed Jobs - 20 0-10-16 | 36543.2 total core 20-09- XDMoD Z |
| 937234.6 i Recently 16 to 202 ID 4274244 | nefficent core hours/16 hours Completed Jobs - 20 0-10-16 Name | 20-09-XDMoD Z |
| 937234.6 i Recently 16 to 202 ID 4274244 [4270864] | nefficent core hours / 16 hours Completed Jobs - 20 0-10-16 Name SimRunArray_12 | 036543.2 total core 120-09- XDMoD Date CPU 10/5 25.5 |



OnDemand - XDMoD job stats





Open OnDemand + Power Al

- Huckleberry
 - 14 node Power 8 cluster
- ECE recruitment tool
- Teaching tool
- Al workhorse
- DeepLearning Hackathons

| reserved/down | | | | | | | | | |
|--|---------------|---------------------------------|--------------------------------|--------------------|----|---|---|------------------------|---|
| nodes | 14 | 14 | 14 | 0 | | 2 | 0 | 0 | |
| cores available | 587 | 523 | 587 | 72 | | 0 | 352 | 376 | |
| gpus available | - | - | - | - | | 8 | 8 | 11 | |
| 1/2 nodes available | 18 | 16 | 18 | 1 | | 0 | 15 | 16 | |
| full nodes available | 17 | 15 | 17 | 1 | | 0 | 0 | 1 | |
| %utilization cores/nodes | 89.6/90.3 | 90.6/91.4 | 4 89.6/90.3 | 3 50/50 | | 100/100 | 61.4/100 | 60.8/97. | 5 |
| Dragonstooth cor 11:20:24AM | | - | | | ; | | v core and node er, 2020 11:2 | 0:24AM | |
| | | dev_q | normal_q | preemptable_ | .q | | | normal_q | |
| total cores/node | • | 24 | 24 | 24 | | | | | |
| nodes in partitio | | | | | | total cores | /node | 20 | |
| nouce in partice | n | 47 | 42 | 47 | | total cores | | 20 4 | |
| reserved/down | | 47 0 | 42 0 | 47 0 | | | /node | | |
| · · · | nodes | | | | | total gpus, nodes in p | /node | 4 | |
| reserved/down r | nodes | 0 | 0 | 0 | | total gpus, nodes in p | /node artition lown nodes | 4 | |
| reserved/down r | nodes able | 0 107 | 0 36 | 0 107 | | total gpus, nodes in p reserved/c | /node artition lown nodes lable | 4 14 3 | |
| reserved/down r cores available 1/2 nodes availa | nodes | 0 107 5 | 0 36 2 | 0 107 5 | | total gpus, nodes in p reserved/c cores avai | /node artition lown nodes lable able | 4 14 3 0 | |
| reserved/down n cores available 1/2 nodes availa full nodes availa %utilization core | nodes | 0 107 5 3 90.5/93.6 | 0 36 2 1 96.4/97.6 | 0 107 5 3 | | total gpus, nodes in p reserved/c cores avai gpus avail | /node artition lown nodes lable able available | 4 14 3 0 0 | |



Huckleberry Power8 AI

Power is just another choice in OnDemand.

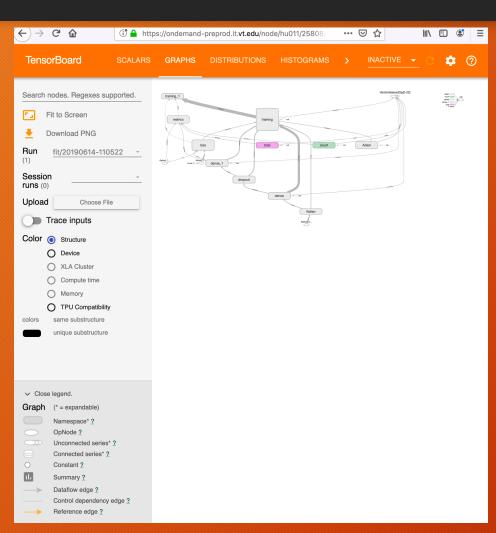
To further enable, we have surfaced the IBM Power AI stack through Anaconda. To facilitate use, allow loading of the environment via Open OnDemand.

Note: traditional ssh; module load; conda activate works!

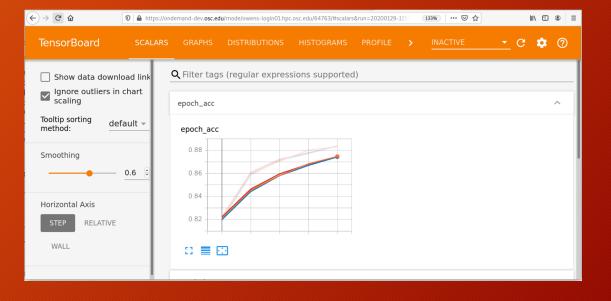
| Interactive Apps | Jupyter Notebook | U) |
|----------------------------------|---|----|
| Cascades | Launch a Jupyter Notebook server on Huckleberry and will activate the | |
| ecre BYO-Container | PowerAl environment. | |
| COMSOL Multiphysics | Account | |
| 😇 Jupyter Notebook | ondemand2 | |
| Supyter Notebook (Julia-enabled) | • The allocation you would like to use for SLURM. | |
| Jupyter NotebookContainer | Reservation | |
| 📣 MATLAB | | |
| III ParaView | Partition | |
| « QGIS | normal_q | |
| Remote Desktop | • To request a GPU enabled queue, preface it with v100 Example: | |
| Studio | v100_normal_q | |
| sww Stata | Number of hours (min-1, max-48) | 0 |
| VisIT | | ۲ |
| Dragonstooth | Number of nodes (min-1, max-2) | |
| - DNAmonitor | 1 | 0 |
| 🥃 Jupyter Notebook | Number of cores per node (min-1, max-20) | |
| 📣 MATLAB | 10 | 0 |
| « QGIS | Number of GPUs per node (min-0, max-4) | |
| ☐ Remote Desktop | 1 | 0 |
| a Rstudio | If requesting GPU nodes, you must enter a GPU-enabled Partition above or the job will fail. | |
| Rst. for STAT3615 | Required modules | |
| Stata | gcc/7.3.0 cuda/10.1.105 jdk/8.0.5.31 Anaconda3/2019.03 | |
| VisIT | This should be spaced list of -compatible- modules. | |
| Huckleberry | gcc/7.3.0 cuda/10.1.105 jdk/8.0.5.31 Anaconda3/2019.03 | |
| 😅 Jupyter Notebook | Conda environment | |
| | powerai16_ibm | |
| Interactive Apps [Sandbox] | • This should be a Conda environment you wish to load. The conda | |



AI/ML/DL benefit from Tensorboards



- Monitor training/learning progress
- Troubleshoot network design





Hackathons, education, new users

- Power + Open OnDemand!!
- Hackathons are short duration learning challenges.
 - Move the focus from platform access to the hackathon topic immediately!!
- Education
 - Don't create the day 1 bottleneck of "how do I ssh to ..."
- New users
 - Gentle introductions, all traditional modes of access are maintained



What types of AI projects are running at VT

- Multi-robot coordination and navigation
- Smart city communications and security
- Crop identification and management
- Physics informed predictive turbulence
- Auto-turning of CFD algorithms
- Prosthetic tuning for walking
- Improvements in communications systems
- Autonomous vehicles

•

• Search and rescue via drone swarms



Power group: Jian-Bin Huang, ECE@VT

Research Goal

Leverage large amounts of visual data that are readily available on the web to learn, understand, and synthesize our visual world.

Teach machines to see!

Motivation

Machine learning (deep learning) models work well if we have

lots of labeled data.

Supervised learning •Not scalable!

Unlabeled data •Readily available!

Our approach

•Use both labeled and unlabeled data for visual learning

Learning Visual Reconstruction

How do we recover the missing data?





Video completion

Learning Dense Correspondence

How do we match and align a pair images?





Stereo matching

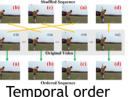
Labeled Datasets

facebook

Motion estimation Semantic correspondence

Learning Generalizable Representation

How do train models that learn new task efficiently?





Lifelong learning

Selected Publications



Open OnDemand: Adoption is growing

- Features:
- Plugin-free web experience
- ✓ Easy file management
- Command-line shell access
- ✓ Job management and monitoring
- Graphical desktop environments
- ✓ GUIs
- Install base is growing
- Industry and academia
- ~140 unique US locations
- ~70 unique international locations

Production Deployments





Center for Computational Research

Ohio Supercomputer Cente



Questions?

Robert Settlage Advanced Research Computing @Virginia Tech Oct 2020





