

HPC at VT

Robert Settlage

Advanced Research Computing

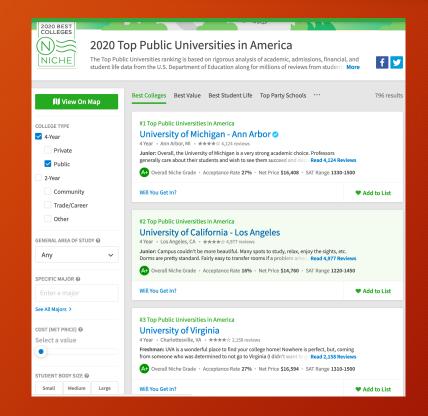
Spring 2020

It's that time of year...



Who am I

- Researcher
- Collaborator
- Educator
- Nvidia DLI Ambassador (CUDA, CV)
- Chemist
- Statistician
- Computational Scientist
- UVA grad and fan



We are Virginia Tech



And well fed

The only school to:

Sequence and assemble the genome 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 * 은 쩓, Aleksey V. Zimin [†], Robert E. Settlage [‡], Sungwon Kim ^{*}, Kent M. Reed

Show more

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

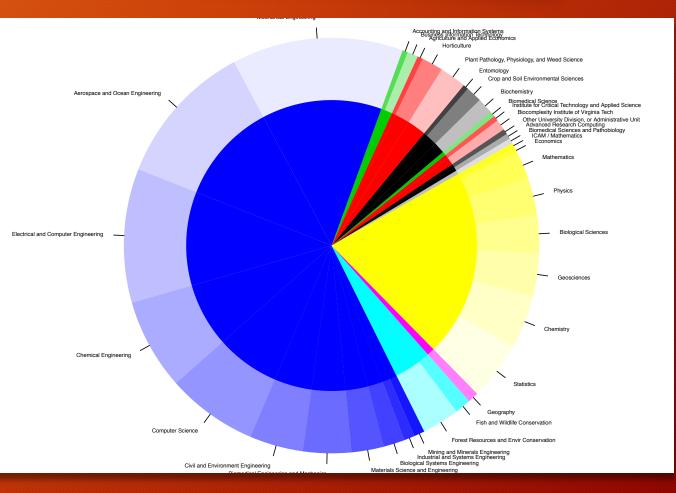




- ARC
- Getting Started on ARC
- Enabling Users with Open OnDemand

ARC - who we are

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



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

Getting started on ARC

Center for Computational Research

versity at Buffalo

What do you need?

- An account
- An allocation

| GINIA Advanced Re | esearch Computing | | |
|---|--|------------------------------------|-----------|
| of Information Technology | | | ٩ |
| USER DA | SHBOARD USER INFO - RESOURCES - NEWS - | ABOUT - SUBMIT A REQUEST - | |
| 11.January 2019 | | ACCOUNT | |
| Advanced Research Computing | | HELP | |
| Jon Tomma Network Preserv Consulty Network Preserve | | CONSULTATION | MA |
| VE VICCHILA | | RESERVE VISUALIZATION RESOURCES | |
| ARC NEWS | ARC NEWS | ARC NEWS | |
| WHAT CAN ARC DO FOR YOU? | NEW ARC CLUSTER : HUCKLEBERRY | GAS-SURFACE INTERACT | TIONS ARE |

ARC.vt.edu

- Requests
- account request

Coldfront.arc.vt.edu

1. Create a project

B Ohio Supercomputer Center

2. Create an allocation

| i 🔒 https://coldfront.arc. vt.edu 🛛 😵 📔 🚥 😒 🏠 | | | | | | |
|--|----------------------------------|------------------|----------------------|--------|--|--|
| ColdFront - Resource Allocation System | | | | | | |
| Home Center Summary Project - Director - Hel | | | | | | |
| 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 | Active | | |
| /groups/inyoungk_lab/ | | sp20 | (Cluster) | | | |
| /groups/arcsingularity/ | Bovine DNA methylation | bDNA | Compute (Cluster) | Active | | |
| | ARC-training | arc-train4 | Compute (Cluster) | Active | | |
| | root | root | Compute (Cluster) | Active | | |

VIRGINIA TECH.

Open OnDemand 2.0

🖺 Archive Project

| Principal Investigator: Robert Settlage (rsettlag) 🖂 |
|--|
| Description: Open OnDemand setup and configuration |
| Field of Science: Advanced Research Computing |
| Project Status: Active |
| Created: Sep. 04, 2019 |

| 📽 Users 🗗 | 2 | | Email Project Users | | | |
|-----------|-----------------------|------------------|---------------------|--------|------------------------|------------|
| Username | Name | Email | Role 🚺 | Status | Enable Notifications 🔒 | Actions |
| bbooker | Brandon Booker | bbooker@vt.edu | User | Active | ۷ | 2/ |
| brownm12 | Matthew Brown | brownm12@vt.edu | User | Active | ۵ | 2/ |
| bsawyers | Brandon Sawyers | bsawyers@vt.edu | User | Active | | ۵. |
| 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 | | ٠. |
| rsettlag | Robert Settlage | rsettlag@vt.edu | Manager | Active | V | ٠. |

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

Student

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

Enabling Users with Open OnDemand

Provides an easy to install and use, web-based access to supercomputers, resulting in intuitive, innovative support for interactive supercomputing

Features:

- Plugin-free web experience
- ✓ Easy file management
- Command-line shell access
- Job management and monitoring
- Graphical desktop environments

✓ GUIs

Production Deployments





Adoption is growing

- Install base is growing
- Industry and academia
- ~140 unique US locations
- ~70 unique international locations



Interested / Evaluating



<section-header> Image: A constrained by the constraine

Enabling Users with Open OnDemand

Open OnDemand

| \$7 7 7 | OnDemand | Files - | Jobs - | Clusters - | Interactive Apps - | My Interactive Sessions |
|----------------|----------|--------------------|--|------------|---|-------------------------|
| | | Home / | My Interactiv | >_Dragonst | s Shell Access tooth Shell Access erry Shell Access | |
| | | ⊜ Jupyte | OL Multiphys r Notebook (r Notebook (B e Desktop | | | active sessions. |
| | | 😅 Jupyte | r Notebook | | | |

| Jupyter Notebook Container (293286) | 1 node 1 core Running |
|--|---------------------------|
| Host: ca200 | Delete |
| Created at: 2020-02-17 14:24:26 EST | |
| Time Remaining: 59 minutes | |
| Session ID: a8d45e4c-8c38-4355-a812-15edf7349805 | |

| Interactive Apps | Jupyter NotebookContainer | | |
|--|---|--|--|
| Cascades | Launch a Jupyter Notebook on Cascades and optionally activate a Conda | | |
| COMSOL Multiphysics | environment. | | |
| Jupyter Notebook | Container set | | |
| Jupyter Notebook (Julia-enabled) | tensorflow-notebook · | | |
| Jupyter NotebookContainer | These Images are pulled directly from the Jupyter Docker Stacks. See | | |
| 📣 MATLAB | here: https://jupyter-docker-stacks.readthedocs.io/en/latest/using /selecting.html#core-stacks | | |
| M ParaView | Account | | |
| « QGIS | ondemand2 | | |
| Remote Desktop | • The allocation you would like to use for SLURM. | | |
| Rstudio | Reservation | | |
| Stata | | | |
| Dragonstooth | Partition | | |
| - DNAmonitor | v100_normal_q | | |
| 👼 Jupyter Notebook | To request a GPU enabled queue, preface it with v100 Example: | | |
| 📣 MATLAB | v100_normal_q | | |
| xx QGIS | Number of hours (min-1, max-48) | | |
| Remote Desktop | | | |
| Astudio | Number of nodes (min-1, max-2) | | |
| Rstudio for STAT3615 | | | |
| - Stata | Number of cores per node (min-1, max-32) | | |
| Huckleberry | | | |
| Jupyter Notebook | Number of GPUs per node (min-0, max-2) | | |
| | 0 | | |
| Interactive Apps [Sandbox] | If requesting GPU nodes, you must enter a GPU-enabled Partition above or the job will fail. | | |
| Cascades | , | | |
| ANSYS Workbench | Conda environment | | |
| COMSOL Multiphysics | This should be a Conda equirement you wish to lead. The conda | | |
| Example Shiny App | This should be a Conda environment you wish to load. The conda environment must contain ipykernel for this to work. Once the notebook | | |
| ≓ Genome Browser | has started, you can type "lwhich python" to make sure you are within your Conda environment. | | |
| 😅 Jupyter Notebook | PYTHONUSERBASE for user install packages | | |
| Jupyter NotebookContainer | | | |
| ▲ MATLAB | This sets the local directory for installing user packages. | | |
| NSIGHT | I would like to receive an email when the session starts | | |
| m ParaView | Launch | | |
| a QGIS | * All Jupyter NotebookContainer session data is generated and stored under the user's | | |

ondemand.arc.vt.edu

Off-campus = VPN

Openondemand.org

Open OnDemand Demo

