Maximizing Your Time with a CBHDS Biostatistician/Bioinformatician Data Transfer and Management

Please consider the following guidelines when using Virginia Tech's <u>Advanced Research Computing (ARC)</u> for data storage. This document is created based on <u>VT ARC documentation</u>. The purpose of this document is to provide general guidelines for the use of ARC for data transfer and management at the Center for Biostatistics and Health Data Sciences (CBHDS). Note that You do not need to have any prior experience with high-performance computing (HPC) to follow this document. **Before you start following the instructions below, please make sure you are connected to VT's network.** If you have trouble with any section of the instructions provided in this document, please email Dr. Missi Zhang at <u>missizxm@vt.edu</u>.

### **ARC Services**

ARC is a unit within VT's Division of Information Technology, providing centralized research computing infrastructure and support the university's research community. VT ARC provides high-performance computing systems, large-scale data storage, big data processing, software, and consulting services. It is designed for researchers from different disciplines or in different locations to collaborate on a project. ARC is very helpful when you have large jobs to run (e.g., high resolution or large-scale datasets), many jobs to run (parameter sweeps, many datasets), or needs for specialty hardware (GPU, memory, high bandwidth storage, fast network, scale). ARC also provides introductory training sessions via the TLOS <u>Professional Development Network</u> and there are computational scientists available in the ARC team to provide the necessary support.

#### For VT Users

ARC is available to all Virginia Tech faculty at no cost. Researchers and groups have the option to add computing costs to grants or contracts through ARC's Cost Center for requesting additional compute or storage resources. Departments and faculty can also purchase priority access to an ARC system for up to five years through ARC's Investment Computing Program.

# Links to ARC References and Additional Resources

- Office Hours
- <u>Request a Consultation</u>
- Create an ARC User Account
- New ARC Users Info
- <u>Video tutorials</u>
- <u>Computing Resources</u>
- <u>Storage Resources</u>
- <u>Visualization Services</u>
- <u>ARC Faculty & Staff Directory</u>

# **Getting Started with ARC**

This section contains instructions for creating user accounts, requesting project storage space and computation allocations, managing projects and user lists, as well as transferring and managing data on ARC. **Before you follow these instructions, please make sure you are connected to VT's campus network.** If you are not using VT's campus network, please use VT's Ivanti Remote Access VPN. Instructions about how to connect to VT's Remote Access VPN can be found <u>here</u>.

# 1. Create an ARC user account.

ARC accounts are based on VT PID accounts and authentication.

- a valid VT PID is required and logins to ARC systems are authenticated with VT PID username and password plus DUO second factor authentication.
- All current faculty, staff, and students at VT have a VT PID.
- Collaborators external to VT can get a "<u>sponsored VT PID</u>" when that is requested by a faculty member at VT.

**Anyone with an active VT PID can request access to ARC system.** The <u>account creation form</u> will require you to confirm your acceptance of VT usage policies, and then create your account. Once your account is created, you can login in ARC.

Next, you will need to create a project and request allocations for this project. An allocation is a system time account requested and managed by a single person (e.g., a project Principal

Investigator [PI]). Many users (e.g., Co-Investigators [Co-I] or graduate students) can then be granted access to a single allocation. There are two types of project allocations:

Research Allocations: for research projects & managed by the project's PI

- Typically granted for a single year and can be renewed annually for the length of the project.
- Multi-year research allocations may be granted through negotiation with ARC.
- Can be used for CBHDS data science projects.

Who is eligible for research allocations?

- a current faculty member or post-doctoral researcher at VT.
- an employee of VT and the PI for a research computing-related project.
- an employee of VT and the Co-I for a research computing-related project led by a non-VT PI Adjunct professors must provide a letter from their department chair, indicating that they are qualified to lead an internal research project, before their project and allocation requests can be approved.

Instructional Allocations: for academic classes & managed by the faculty member/instructor

- typically smaller, available for shorter time periods
- limited to a select set of systems.
- Can be used for training workshops.



*Figure 1.1. The relationship between project allocation type and function.* 

# 2. Create a new project.

Once your ARC account is approved, you can go to <u>ColdFront</u> to create a project, add users, request allocations, and add grant/publication information.

- 2.1. Log into <u>ColdFront</u> using your ARC account username and password.
- 2.2. On the home page, your username should appear on the top right corner (as depicted in Figure2.1 below). To create a new project, click "Projects" and then click "Add a project".

Cold Front	ARC	
Home Center Summar	y Project • Help	<b>د ا</b>
		۲ Your username
+ Add a project		View archived projects
Projects		

*Figure 2.1. The home page of ColdFront.* 

2.3. In order to create a project, you will need to fill and submit the following form below with information on the project title, description, and your department.

Title*	
Description*	Please fill out this field.
We do not have in	ormation about your research. Please provide a detailed description of your work and update your field of science. Thank you!
Department*	
Center for Biostati	tics & HDS
Save Cancel	

Figure 2.2. A project request form.

- 3. Set up new allocations.
  - **3.1.** Once you have created a new project, log into <u>ColdFront</u> using your ARC account username and password to set up new allocations.
  - **3.2.** On the home page, you will see the recently created project on the project list on the left. Click the project title/name to visit the project management page.
  - 3.3. In order to authorize a student or a lab member to access your project, please click "Add

Users" as shown in Figure 3.1. Then use a VT PID username or email address to find and add this person to your user list.

The authorized users include regular users and project managers. Managers are allowed to grant user access and edit the project information.

ColeFront ARC		
Home Center Summary Project - Help		💄 PID username 🔻
Project Title		
& Manage Project	C Update Project Information	Archive Project
Add Users 🗣 Add Grant 🛛 🖬 Add Publication 🗐 Add Research Output		
Principal Investigator: PI's full name (PI's username) 🖂		
Description: Project Description		
Department: Center for Biostatistics & HDS		
Project Status: New		
Created: Aug. 23, 2023		

*Figure 3.1. A project management page.* 

**3.4.** To request storage and computational resources, please click the "Request Resource Allocation" as shown below in Figure 3.2 and select the allocation type.

Then you'll need to fill out two forms. "Storage allocation" is for requesting project storage space, and "compute allocation" is for requesting computation resources. ARC provides 0.6 million core-hour/month and 25TB storage for free to all VT PIs. Extra storage space and computation time can be granted upon request at a <u>cost</u>.

Allocations 2	+ Request Resource Allocation
Show 10 ¢ entries	Search:
Resource Name 🔨 Resource Type 🛝 Information	∿ Status ∿ End Date ∿ Actions

*Figure 3.2. Requesting resource allocations for a project.* 

You will need to select the allocation type. Please revisit Section 1 of this document for details

on allocation types.

# **Request New Allocation**

Project: Bioinformatics-CBHDS

The following ARC resources are available to request for this project. If you need access to more than one of these, please submit a separate allocation request for each resource. For each request you must provide the justification for how you intend to use the resource to further the research goals of your project.

Resource*
Compute (Free) (Cluster)
Justification*
Tell us what your resource requirements are.
Justification for requesting this allocation.
Core hours (up to 800k/month) (TinkerCliffs only, no monthly usage limits on other clusters)*
800000
Users  Select All Users
Select users in your project to add to this allocation.
Select account name to associate with resource. Click here to create an account name
Allocation type*
<ul> <li>esearch</li> <li>○ instructional</li> </ul>
□ I have uploaded the relevant publication and grant information*
Submit Back to Project

Figure 3.3. Requesting computing hours for a project.

Please click the circled line "Click here to create an account name!" to create an account name. This is your slurm account name. You and the authorized users on the project user list will need this account name for running data analysis jobs on ARC.

# **Request New Allocation**

#### Project: Bioinformatics-CBHDS

The following ARC resources are available to request for this project. If you need access to more than one of these, please submit a separate allocation request for each resource. For each request you must provide the justification for how you intend to use the resource to further the research goals of your project.

Project (Free) (Storage)	
ustification*	
<b>T</b> II	
Tell us what your resource requirements are.	
Justification for requesting this allocation.	
Terabytes (first 25 TB free. Click here for more details)*	
0	
Jsers	
Jsers Select All Users	
Jsers Select All Users	
Jsers Select All Users Select users in your project to add to this allocation.	
Jsers Select All Users Select users in your project to add to this allocation.	
Jsers Select All Users Select users in your project to add to this allocation. Select account name to associate with resource. Click here to create an account name!	
Jsers Select All Users Select users in your project to add to this allocation. Select account name to associate with resource. Click here to create an account name!	
Jsers Select All Users Select users in your project to add to this allocation. Select account name to associate with resource. Click here to create an account name! Allocation type*	
Jsers Select All Users Select users in your project to add to this allocation. Select account name to associate with resource. Click here to create an account name! Allocation type* research instructional	
Jsers Select All Users Select users in your project to add to this allocation. Select account name to associate with resource. Click here to create an account name! Allocation type* research instructional Lawe uploaded the relevant publication and grant information*	
JSers Select All Users Select users in your project to add to this allocation. Select account name to associate with resource. Click here to create an account name! Allocation type* research instructional I have uploaded the relevant publication and grant information*	

#### 4. Manage ARC projects.

- 4.1. To manage ARC accounts and project directories (folders), please go to ColdFront.
- 4.2. On the home page, you'll see a project list on the left. All projects provided to you in this list are the ARC projects that you currently have access to.
- **4.3.** To find and review the specific information of a project, simply click the name of that project (Figure 4.1.):



*Figure 4.1. Reviewing your projects on the ColdFront home page.* 

# 4.4. You add or remove users and request additional storage and computational resources on the project management page.

Once you enter the project management page, scroll down to the "users" and "allocations" sections to manage the user list and find the account information. The project directory path is also shown in the "allocations" section. The authorized users include regular users and project managers. Managers are allowed to grant user access and edit the project information.

📇 Users 🛛	)		🖾 Email P	roject Users	<b>≗</b> + Add User	s 💄 🔺 Re	move Users		
Username	Name	Email		Role 🚯	Status	Enable	Notifications (		Actions
				Manager	Active				<b>2</b> /
				Manager	Active				2/
				Manager	Active				<b>2</b> /
Allocatio	ons 🛛						+ Reque	est Resourc	e Allocation
Show 10 \$ ent	ries						Search:		
Resource Name	₩	Resource Type 🛛 🛝	Information			∿ Statu	is 🛝 End D	ate 🛝	Actions
Compute (Free)		Cluster	slurm_accou	nt_name:		Active	e 2025-	-06-07	B
Project (Free)		Storage	/projects/cbh	nds-bioinfo/ (25	TB)	Active	9		
Showing 1 to 2 of 2	2 entries		i ne project	directory path				Previous	1 Next

*Figure 4.2. User and allocation management on the ColdFront project management page.* 

## 4.5. To access your project on ARC, please go to the project web page on Open OnDemand.

All the authorized users on the user list of a project have access to the corresponding project directory. Note that newly added users will acquire immediate access to a project through the terminal (Command Line Interface, CLI), but it takes longer to activate the GUI (Graphic User Interface) access.

ARC Open OnDemand	Apps - Files -	Jobs -	Clusters -	Interactive Apps -	IDE -	My Interactive Sessions			<b>0</b> H	elp - 🛔	Logged in as	your username	🕞 Log Out
							>_ Open in Terminal > + New Fi	le 🛛 🖿 New Direct	ary 🛓 U	pload 🛃	Download 🚺	Copy/Move	Telete
Harry Directory							click "Open in Temrinal" to						
Projects			•	/ projects / cbhds-b	ioinfo /	Change directory							Copy path
								Show Owner	/Mode	Show D	otfiles Filter Showing	: 4 rows - 0	rows selected
				Туре	Name		*.	Size	÷, в	Modified a	it		
				•	cbhds	_bioinformatics_projects	<b>!</b> •	-	7	/19/2024	1:59:40 PM		
				•	data_	submission	:*		8	3/11/2023 1	12:46:46 PM		
				•	READ	ME	I -	-	8	3/11/2023 1	11:25:23 AM		
				•	works	hop	I •	-	ε	3/11/2023 1	10:51:16 AM		
Moat Unkercliffs1 arc.vt.edu Initial dir (@tinkercliffs1 cb	ectory:/projects/obhds-blo hds−bioinfo]\$	Dinto									Themes:	Default	V

*Figure 4.3. Entering the Command Line Interface (bottom) from the Graphic User Interface (top) of an ARC hpc cluster.* 

#### 5. Data Transfer and Management

If you cannot have an ARC account, please contact a CBHDS bioinformatician to submit your data in a different way.

# 5.1. Connect to VT's campus network and grant a CBHDS bioinformatician access to your project directory (following <u>Steps 4.1 through 4.4</u>).

# 5.2. Go to ARC Open OnDemand.

Once you log in using your VT credentials (PID and password), you will see your username at the top right corner of the dashboard (home page) of <u>ARC Open OnDemand</u>. OnDemand provides multiple features including file management and transfer, job management, shell access, and interactive apps. For data transfer, please go to "Files" and then click "Projects" (Figure 5.1.).

ARC Open OnDemand Apps -	Files Jobs - Clusters - Interactive Apps - IDE - IDE - My Interactive Sessions	😯 Help 🝷	Logged in as
	Home Directory  Projects (projects)		Your username
	<b>D</b> nDemand		
	OnDemand provides an integrated, single access point for all of your HPC resources.		
	Message of the Day		
	This system is for authorized users only. Users accessing this system consent to the monitoring, recording and/or disclosure of all activity while using this system.		
	Usage of this system is subject to the terms of the Virginia Tech Acceptable Use Guidelines		
	Pinned Apps A featured subset of all available apps		
	Files		
	Home Directory System Installed App		

*Figure 5.1. Accessing ARC projects from ARC Open OnDemand.* 

5.3. Once you enter <u>the project web page</u>, you will see a list of project directories or folders (Figure 5.2.). To submit data to CBHDS bioinformatics, please go to your project directory. In this case, we will use "cbhds-bioinfo" as an example. Click the project name to enter the project directory.

ARC Open OnDemand Apps - Files - Jobs -	Clusters -	Interactive	Apps 🔹 IDE 👻 🗐 My Interactive Sessions	🖓 Help 👻 🚢 Logged in as 🚺 🚺 Log Out
				>_ Open in Terminal + + New File B New Directory 2. Upland Download @ Copy/Move Directory
Home Directory Projects	1	/ projects /	C Change directory	Copy path
				Show Owner/Mode Show Dotfiles Filter:
				Showing 436 rows - 0 rows selected
		Туре о	Name	*. Size Modified at
		•	179053	: - 7/12/2023 6:24:02 PM
Please scroll down to		•	2019s_cs4884	- 1/9/2024 5:44:15 PM
find "cbhds-bioinfo"		•	2023collakovatomato	
Ļ		•	2023gbcb5874	- 12/13/2023 5:56:49 PM
		•	3dbio	12/13/2023 4:41:58 PM
		•	cbhds	
		- (	cbhds-bioinfo	: - 8/23/2023 12:26:12 PM
		-	cbhds-derekkaknes	- 10/11/2022 8:56:45 AM

Figure 5.2. The project web page of ARC Open OnDemand.

After you enter your project directory, please click "new directory" to create a new directory and name it "data\_submission" (Figure 5.3.).

	>_ Open in Terminal + + New File New Directory	Upload 🛃 Download 🕒 Copy/Move 👕 Delete
		Copy path
	Show Owner/Mode	Show Dotfiles Filter:
		Showing 4 rows - 0 rows selected
Type * Name *	Size Modified at	Owner Mode
Figure 5.3. creating a new directory.		

Click the name "data\_submission" to enter this directory (Figure 5.4.).

1	/ projects / cb	bhds-bioinfo / 🕼 Change directory			Copy path
				Show Owner/Mode	Show Dotfiles Filter: Showing 4 rows - 0 rows selected
	Туре	*, Name	* 	Size	Modified at
0	•	cbhds_bioinformatics_projects	: -	-	7/19/2024 1:59:40 PM
	•	data_submission	: -	-	8/11/2023 12:46:46 PM
	•	README	•	-	8/11/2023 11:25:23 AM
	•	workshop	: -	-	8/11/2023 10:51:16 AM

Figure 5.4. The "data\_submission" subdirectory located in our project directory, "cbhds-bioinfo".

5.4. Once you enter the "data\_submission" directory, you can click "new directory" to create another new directory. Please name this new directory use the format of last name and first & middle name initials, and the data type. For example: "Zhang-XM\_RNASEQ". Next, please click ">\_Open in Terminal" (Figure 5.5.).

				>_ Open in Terminal >	+ New File	New Directory	🔔 Upload	🛓 Download	Copy/Move	🖥 Delete
/ projects	/ cbh	ds-bioinfo / data_submission /	Change directo	ry ]					[1	ி Copy path
						Show Owner/Mc	ide 🗆 Shi	ow Dotfiles F	ilter:	
								Sho	wing 1 rows - 0	rows selected
Туре	*	Name			*	Size	۵ <sup>۸</sup> ۷	Modified at		
•		LastName-FirstMiddleNameIni	tials_TypeOfData			-		8/11/2023 12:	46:46 PM	

*Figure 5.5. creating a raw data directory and entering the terminal interface.* 

5.5. Then you will see a terminal (Command Line Interface) window similar to Figure 5.6.



*Figure 5.6. Shell access to the tinkercliffs1 cluster.* 

5.6. Type "Is (space)-Ih" and hit the "enter/return" key on your keyboard, and you should see

your new directory (Figure 5.7.).



Figure 5.7. Listing the files and folders available in your current directory "data\_submission".

5.7. Now type "chmod (space)u=rwx,g=r,g-s,o= (space)LastName-

FirstMiddleNameInitials\_TypeOfData/ ". Please replace FirstMiddleNameInitials\_TypeOfData with your directory name. Then hit "enter/return".

5.8. Type "Is (space)-Ih" and hit the "enter/return".

Notice the output in the first column changed to "drwxr-----" from "drwxr-sr-x"? Now, everything in this new directory is fully accessible to you and it's readable and downloadable to the CBHDS bioinformatics team.

[username @tinkercliffs1 data_submission]\$ ls -lh
total 1.0K
drwxr-sr-x 2 username arc.cbhds-bioinfo 4.0K Aug 7 15:06 LastName-FirstMiddleNameInitials_Type0fData
<pre>L usemame @dinkercliffs1 data_submission]\$ chmod u=rwx,g=r,g-s,o= LastName-FirstMiddleNameInitials_lype0tData/</pre>
[ username @tinkercliffs1 data_submission]\$ ls -lh
drwxr 2 username arc.cbhds-bioinfo 4.0K Aug 7 15:06 LastName-FirstMiddleNameInitials_Type0fData
l <mark>usemane o</mark> @tinkercliffs1 data_submission]\$

*Figure 5.8. Changing the accessibility of a directory.* 

5.9. Go back to the webpage to confirm that the mode of your directory is "740". Now, you can click "Upload" to upload your data to the directory you just created (Figure 5.9.).

ARC Open OnDemand Apps -	Files • Jobs •	Clusters -	Interactive Ap	ps 👻 IDE	<ul> <li>My Interactive</li> </ul>	Sessions					🕜 Help 👻	Logged	l in as	G Log	g Out
							>_ Open in	Terminal +	+ New File	Ra New Directory	1. Upload	🛓 Download	Copy/Mov	e 👕 Dele	ate
Home Directory Projects		•	/ projects / cl	hds-bioinfe	o / data_submission /	Change direct	tory							🖞 Сору р	bath
										Show Owner/N	ode 🗆 Sho	w Dotfiles	Filter:		
												Sł	nowing 1 rows	0 rows se	elected
			Туре 🔭 🛛	lame				•,	Size	Modified	at	*	Owner "	Mode	λ. v
			-	astName-F	irstMiddleNameInitials	s_TypeOfData		:.	-	8/7/2024	3:06:45 PM			740	

*Figure 5.9. Ready to upload the data files.* 

Note that it is highly recommended to change the directory permission (<u>Step 5.4-5.8</u>) before uploading your data. Changing the permission to "drwxr----" ("740" permission mode) will ensure that you have the full access to your raw data while our CBHDS bioinformatics team can only read or download those files.