CyVerse Documentation

CyVerse

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CHAPTER 1

Goals

- Introduce NEON scientists and staff to CyVerse and its resources.
- Demonstrate via hands-on exercises the CyVerse Data Store, Data Science Workbench (Discovery Environment), Cloud (Atmosphere), BisQue image analysis, Data Commons, and Powered By features.
- Open discussion about how NEON staff or academic scientists working with NEON data could begin to utilize CyVerse at scale.

Suggested topics:

- Identify NEON's computational and data storagelsharing bottlenecks that CyVerse can ameliorate.
- Identify missing components from the current CyVerse infrastructure that NEON requires.

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1.1 Morning Workflow

Description:

First things first - getting enrolled with CyVerse and setting up laptops.

There will be several short remote presentations about the different facets of CyVerse. Each section will include a question and answer session, and hands on material to get you used to working with the tools and services which are available.

1.1.1 Remote Presentations and Presentors

08:30 - 08:45 Overview of the day, schedule, logistics - Tyson Swetnam

08:45 - 09:30 "A History of CyVerse (née The iPlantCollaborative)" - Nirav Merchant, CyVerse Co-PI, Director Data7 Institute University of Arizona.

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09:30 - 10:00 "CyVerse Data Store" - Tony Edgin, Senior Sofware Engineer Core Software, CyVerse.

10:00 - 10:15 Break

10:15 - 11:15 "CyVerse Discovery Environment" - Sriram Srinivasan, Lead Software Engineer Core Software CyVerse; "Apps in Discovery Environment" Upendra Devisetty Ph.D., Science Team Informatician, CyVerse.

11:15 - 12:00 "The Agave API" - John Fonner Ph.D., Research Associate, Texas Advanced Computing Center

Platforms

Topic	Description	Outcome
Data Store	Data Creation, Transfer,	CyberDuck, iCommands, and WebDav
	Sharing	
Discovery Envi-	Data, Apps, Workflows	Sharing/viewing, non-interactive app creation, workflows and
ronment		pipeline creation, VICE.
Agave	Clients, Workflow Cre-	ToGo, Clients, REST API
	ation	

Expected Outcomes

- Learn the history of the iPlantCollaborative, which led to CyVerse, as overview of the last 10 years of the project. Learn about the present impacts of the project, and future directions we are headed.
- Learn how to move data in and out of the CyVerse Data Store, host data publically, and introduce the iRODS iCommands interface.
- Learn how to utilize the data science workbench (Discovery Environment): how to create non-interactive apps using Docker, for running individual jobs as well as pipeline workflow execution. Learn about the Visual Interactive Computing Environment (VICE) for launching common scientific IDE (RStudio, Shiny, Jupyter Lab, Ubuntu Desktops).
- Introduction to Agave and how it utilizes High Throughput Computing and High Performance Computing for a 'bring your own compute' platform.

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1.2 Afternoon Workflow

Learning Center Home

Description:

The afternoon session will continue to introduce CyVerse cyberinfrastructure platforms, including Atmosphere and BisQue; as well as the Data Commons - a platform for hosting published scientific data.

We will demonstrate some example use-cases involving CyVerse and other NSF funded resources.

The day will conclude with a discussion of how to collaborate with CyVerse through our Extended Collaborative Support service, Powered By features, and examples of Federation.

1.2.1 Remote Presentations and Presentors

13:00 - 14:00 "Atmosphere" - Edwin Skidmore, Director, Infrastructure University of Arizona.

14:00 - 15:00 "BisQue & Data Commons" - Ramona Walls Ph.D., Research Associate Professor, University of Arizona

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15:00 - 15:15 Break

15:15 - 15:45 "Example Use Cases" - Open Science Grid, Mats Rynge, USC Information Sciences Institute.

15:45 - 16:15 Jason Williams Assistant Director, Cold Spring Harbor.

16:15 - 17:00 "Extended Collaborative Support, Powered by, & Federation" - Tyson Lee Swetnam, Nirav Merchant

Platforms

Topic	Description	Outcome	
Atmosphere Virtual Machines, Image Creation, Software Installa-		Atmo Web client, Atmo CLI, Open-	
	tion	Stack	
BisQue	Imagery, Analysis	Sharing/viewing images, Archival	
Data Com-	Data, Publication	DOI, metadata	
mons			

Expected Outcomes

- Understanding of how to launch Virtual Machines using Atmosphere Browser UI, CLI, and examples of cloud-native-technologies using CyVerse cloud resources.
- Basic operations in BisQue for image analysis and viewing.
- Understanding of how to use the Data Commons for published scientific research
- Learn about other large data intensive science applications with lessons learned.
- Understanding of how to start more comprehensive collaborative effort with CyVerse.

Description of output and results

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CHAPTER 2

Prerequisites

2.1 Downloads, access, and services

In order to complete this tutorial you will need access to the following services/software

Prerequisite	Preparation/Notes	Link/Download
CyVerse account	You will need a CyVerse account to complete this	Register
	exercise	
Atmosphere access	You must have access to Atmosphere	Request Access
CyVerse Data Store allocation in-	You must be registered for CyVerse	Request Increase
crease (Optional)		(form #2)
Jetstream access (Optional)	You must have registered with XSEDE	Request Access
Cyberduck (Optional)	Standalone program for uploading/downloading	Download
	data to Data Store	
Windows 10 Linux Subsystem (Op-	Install Ubuntu Bash on a Windows OS	Installation Instruc-
tional)		tions
iCommands Installation (Optional)	Install iCommands for Linux, Windows, or Mac	Installation Instruc-
	OSX	tions

2.2 Platform(s)

We will use the following CyVerse platform(s):

Platform	Interface	Link	Platform Documen-	Quick
			tation	Start
Data Store	GUI/Command line			
Discovery Environ-	Web/Point-and-click			
ment				
Atmosphere	Command line (ssh) and/or Desktop			
	(VNC)			
BisQue	Web/Point-and-click and/or Command-			(See Man-
	line (API)			ual)
DNA Subway	Web/Point-and-click		(See Guide)	
SciApps	Command-line (API)		(See Guide)	
Agave API	Command-line (API)			

2.3 Application(s) used

Discovery Environment App(s):

App name	Ver-	Description	App	Notes/other
	sion		link	links
Muscle	3.8.31	Multiple sequence aligner		
Jupyter-Lab	0.0.3	Base Jupyter Lab Image		
RStudio Geospa-	3.5.0	Based on Rocker Geospatial RStudio Image		
tial				
Shiny Apps	1.5.9	R Shiny with Geospatial dependencies (GDAL,		
		GEOS, etc)		

Atmosphere Image(s):

Image name	Ver-	Description	Link	Notes/other
	sion			links
CyVerse CentOS 6.8 GUI	1.0	base image CentOS 6.8 with GNOME		
Base		GUI		
Ubuntu 18.04 GUI XFCE	1.0	base Ubuntu 18.04 with GNOME GUI		
Base				

2.4 Input and example data

In order to complete this tutorial you will need to have the following inputs prepared

Input File(s)	Format	Preparation/Notes	Example Data

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