

Getting Started with Partek Flow



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Partek Flow Bioinformatics Biowulf Globus Data transfer from NCI CCR Sequencing Facility

As far as the documentation goes, it should say that the licenses are NCI only. People can send a message if they want to ask beyond that.

Getting Started with Partek Flow at NIH

Learning Objectives

After this class, participants will

- Know how to acquire access to Partek Flow
- Become familiar with approaches for transferring data to the NIH Partek Flow server such as Globus
- Be able to import data into a Partek Flow project

What is Partek Flow?

Partek Flow is a point-and-click software and is suitable for those who wish to avoid the steep learning curve associated with analyzing sequencing data through command line and/or code. It enables the analysis of high dimensional multi-omics sequencing data including DNA, RNA, single cell RNA, ATAC/ChIP, and spatial transcriptomics. At NIH, Partek Flow is hosted on the Biowulf High Performance Computing (HPC) cluster. Researchers interact with Partek Flow through a web browser using a URL supplied by Biowulf after a Biowulf and Partek Flow account has been established. This enables investigators to take advantage of the compute power offered by HPC while using a graphical user interface to construct a sequencing data analysis workflow. Partek Flow also enables the creation of publication quality visualizations.

Note

NCI holds a license for Partek Flow.

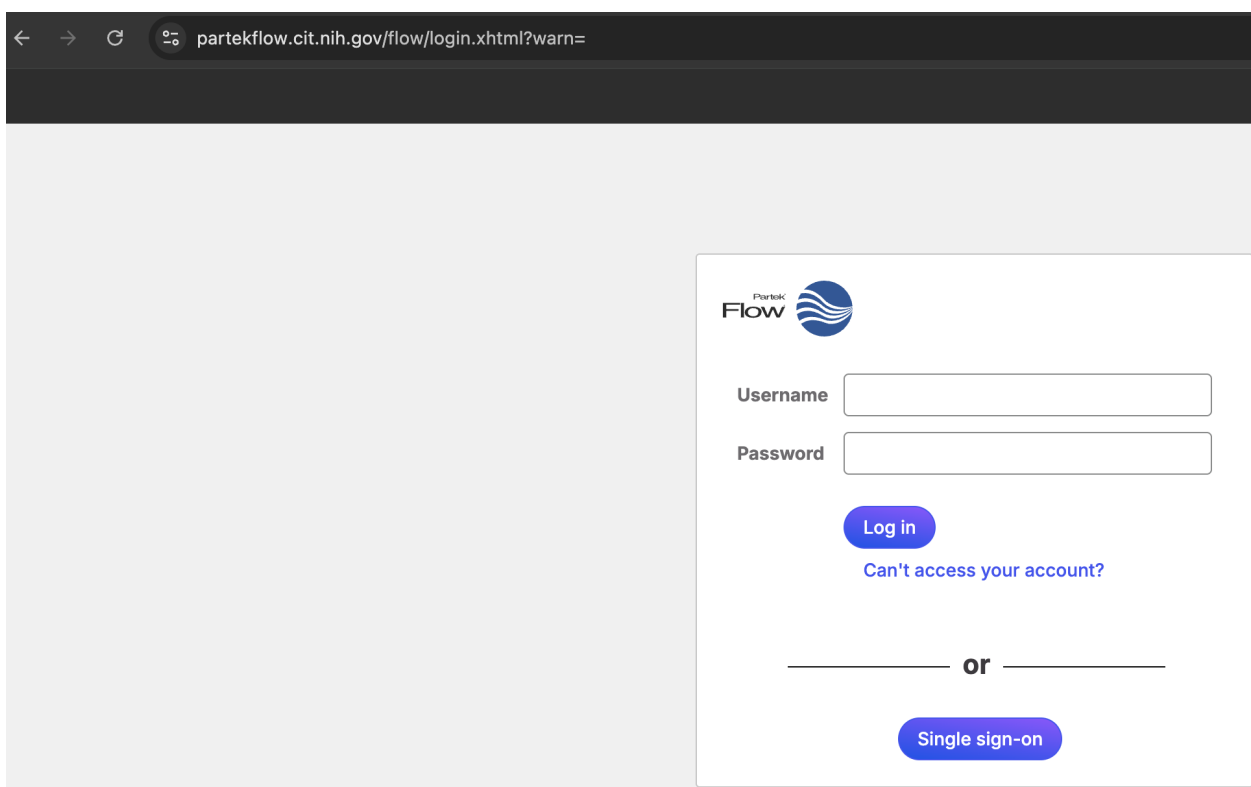
Instructions for Obtaining Access to Partek Flow

NCI researchers can find instructions for accessing Partek Flow at <https://bioinformatics.ccr.cancer.gov/btep/partek-flow-bulk-and-single-cell-rna-seq-data-analysis/> (<https://bioinformatics.ccr.cancer.gov/btep/partek-flow-bulk-and-single-cell-rna-seq-data-analysis/>). Here is what is needed:

- Biowulf (The High Performance Computing cluster) account — [see here for information about how to obtain a HPC account](https://hpc.nih.gov/docs/accounts.html) (<https://hpc.nih.gov/docs/accounts.html>).

- /data directory on Biowulf with enough disk space to hold their Partek Flow files — please fill out [this online form \(https://hpc.nih.gov/dashboard/storage_request.php\)](https://hpc.nih.gov/dashboard/storage_request.php) if you require more disk space.
- Partek Flow account — please contact staff@hpc.nih.gov.

Once these steps have been accomplished, use <https://partekflow.cit.nih.gov/flow> (<https://partekflow.cit.nih.gov/flow>) to sign onto the NIH Partek Flow server. NIH single sign-in enables users to authenticate and connect to the Partek Flow server. Alternatively, users can log on by supplying username and password. However, the password may differ from the one in which the user signs connects to Biowulf with as HPC staff allow for the researcher to set up something different upon Partek Flow account creation. The username though, is the user's NIH username.

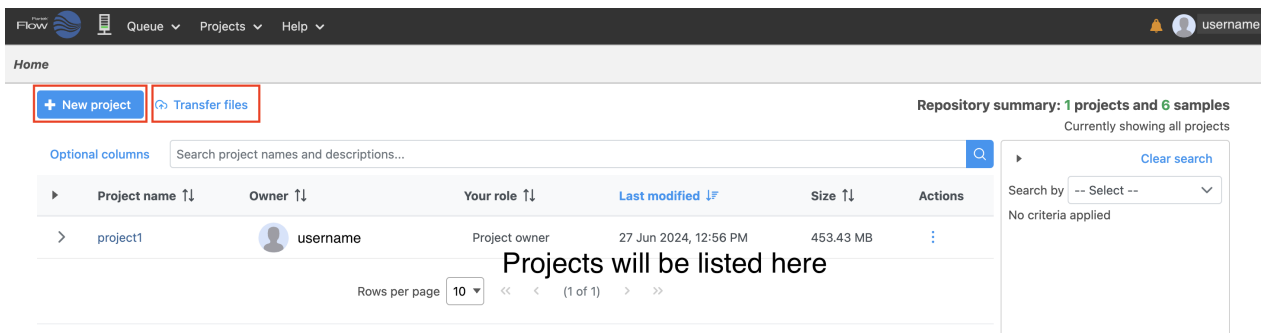


The screenshot shows a web browser window with the address bar displaying `partekflow.cit.nih.gov/flow/login.xhtml?warn=`. The main content area features a login form with the Partek Flow logo at the top. Below the logo are two input fields labeled 'Username' and 'Password'. A blue 'Log in' button is positioned below the password field. Below the button is a link that says 'Can't access your account?'. A horizontal line with the word 'or' in the center separates this from a blue 'Single sign-on' button at the bottom.

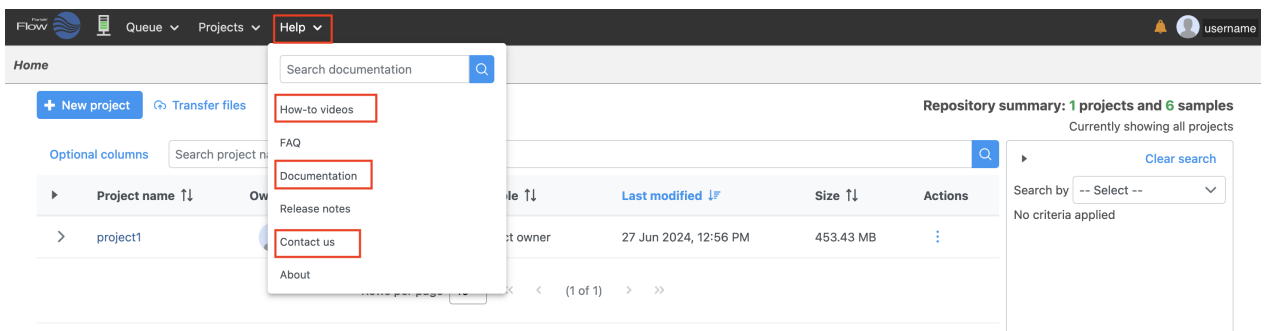
Overview of the Partek Flow User Interface

Upon logging in, users will be taken to Partek Flow's main page. In this page users can access

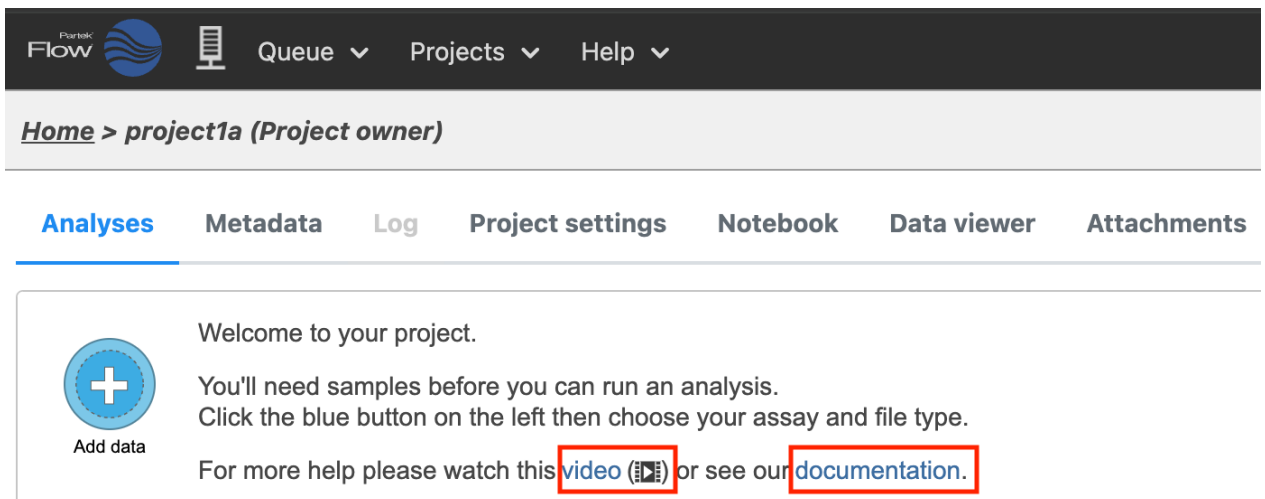
- Help
- View a list of existing projects
- Create new project
- Transfer files (this does not use Globus)
- Access user profile



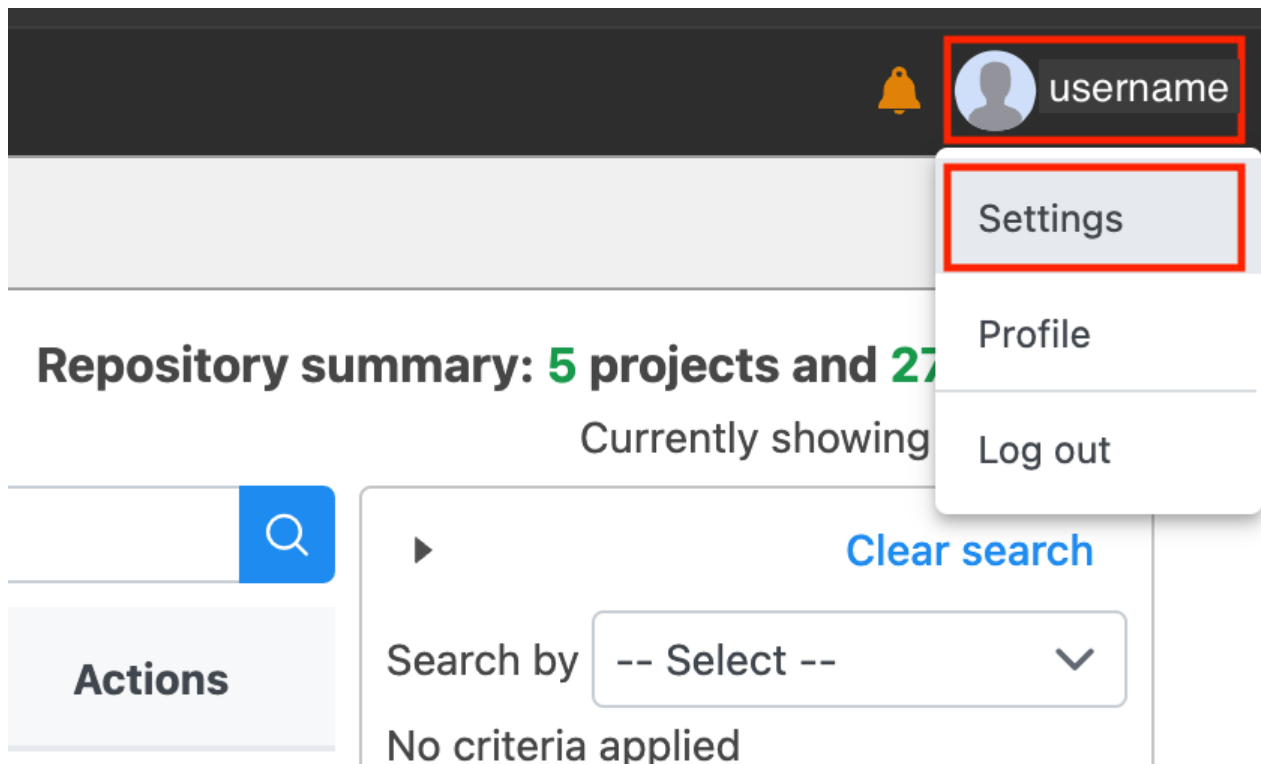
Users can access help documentation, how-to videos and information for contacting support under the "Help" menu. The email for Partek support is support@partek.com.



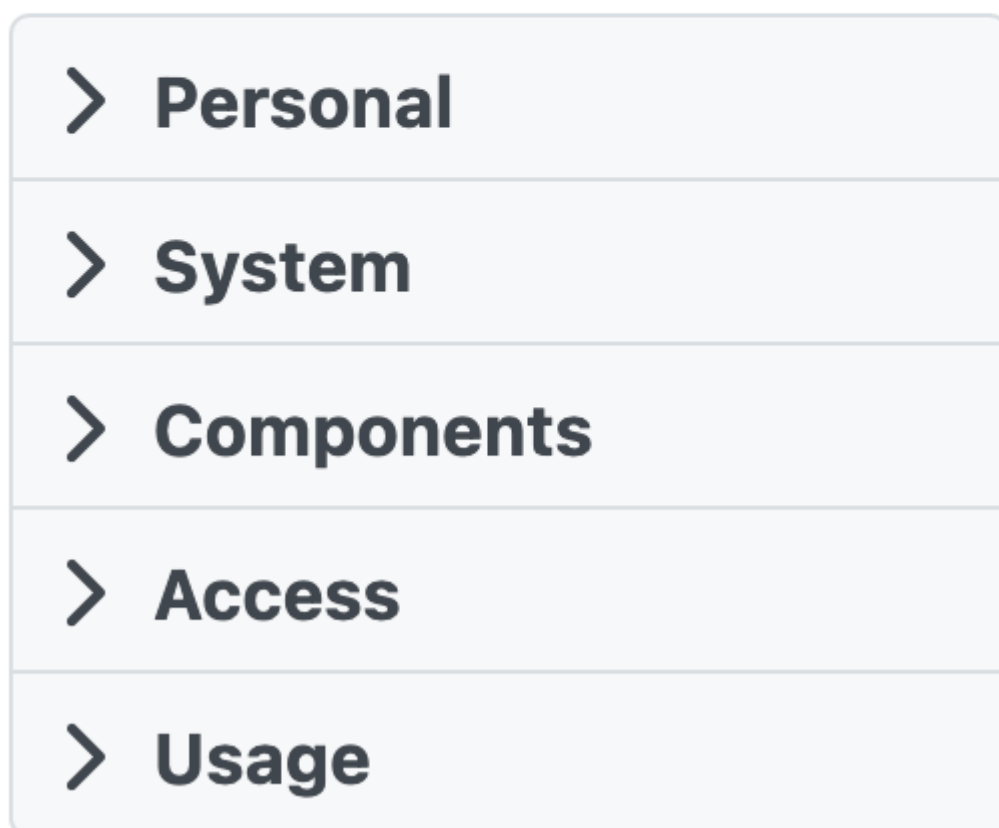
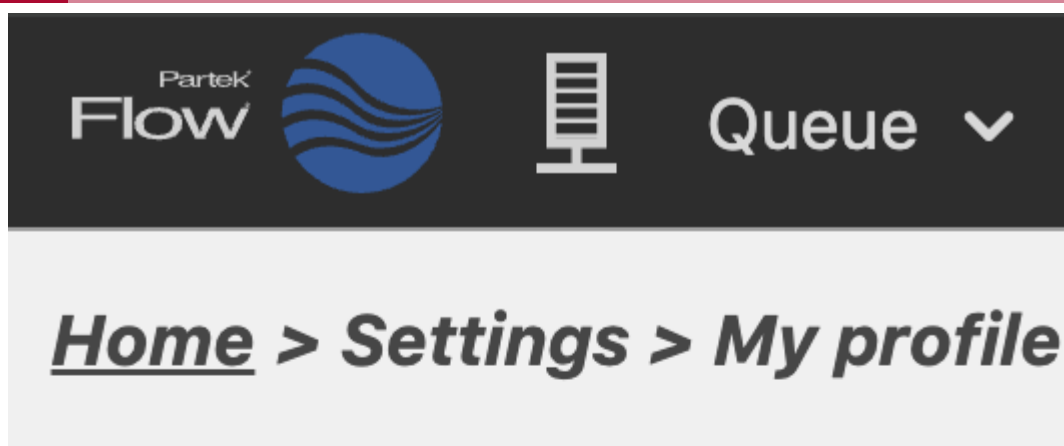
Where applicable, users can find links to how-to video and documentation for specific tasks, such as importing data.





The settings section is divided into five tabs, which are expandable to reveal more options.



Click on the user profile tab at the top right to reveal the option for changing settings.



User profiles can be viewed and edited under "My Profile" in the "Personal" settings section. Note the information regarding the user's Biowulf /data folder storage usage and quota.

  Queue ▾ Projects ▾ Help ▾

[Home](#) > [Settings](#) > [My profile](#)

▽ Personal

[My profile](#)

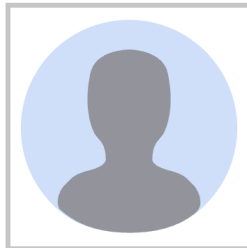
My preferences

> System

> Components

> Access

> Usage



[Change image](#)

Display name username

Username username

Email first.last@nih.gov



Password

Disk usage 103.16 GB (3% of 3.00 TB quota)

[Edit details](#)

Users can access an example bulk and single cell RNA sequencing dataset under the "System" setting tab.

An important feature in the settings is that users can manage genomic references and annotations by clicking on "Library files" under "Components".



Queue ▾ Projects ▾ Help ▾

[Home](#) > [Settings](#) > [Library files](#)

Personal

My profile

My preferences

System

System information

Components

Library files

Lists

Pipelines

Filters

Option sets

Installed tasks

Data repository

Access

Usage

System queue

System resources

Genomic library files

Prep kit files

Other library files

Assembly

Aegilops tauschii - Aegilops tauschii ▾

Reference files ⓘ

+ Add reference files

Library file	Owner	Ignore	Actions
Reference sequence	owner	<input type="checkbox"/>	⋮

Reference aligner indexes ⓘ

+ Add reference aligner indexes

Library file	Owner	Ignore	Actions
Bowtie index	owner	<input type="checkbox"/>	⋮
Bowtie 2 index	owner	<input type="checkbox"/>	⋮
HISAT2 2.1.0 index	owner	<input type="checkbox"/>	⋮

Users can view "Systems resources" under the "Usage" settings. Here, users are informed of how many tasks are running and waiting in the queue. A visualization of Biowulf Partek Flow worker nodes is also provided.

partekflow.cit.nih.gov/flow/settings/resource-management.xhtml

Partek Flow Queue Projects Help

[Home](#) > [Settings](#) > [System resources](#)

> Personal

> System

> Components

> Access

▼ Usage

System queue

System resources

[View queued tasks](#)

Queue status

[Running tasks](#) 1

[Waiting tasks](#) 0

Time estimates are being continuously updated and will become more accurate.

Active workers

Name	CPU usage	Memory usage	Machine capacity	Uptime	Type
hpcpartek.cit.nih.gov			12 cores 63 GB RAM		Server
cn2287	 load w: 0.0 s: 0.0	 w: 0.0 s: 7.3 GB	56 cores 252 GB RAM	1 day	Worker
cn3168	 load w: 1.0 s: 0.0	 w: 5.6 s: 8.0 GB	56 cores 252 GB RAM	07:55:54	Worker

Worker usage
 System usage
 Worker limit

Licensing

[Available worker licenses](#) 48 out of 50

Class overview slides

I

Tips on Biowulf for Partek Flow Users

Even though Partek Flow runs on Biowulf, the NIH Unix-based high performance computing cluster, users do not need to be experts in command line to use this software. However, there are some things that are useful to know because Partek Flow projects, input, and output are all stored on Biowulf.

Signing onto Biowulf

To sign onto Biowulf, open a Terminal if using MacOS or Command Prompt if using Windows 10 or above. Once opened, at the prompt, do the following to sign on. The breakdown of the command is as follows.

- `ssh`: Connect to remote computer (ie. Biowulf)
- `user`: User's NIH username
- `@biowulf.nih.gov`: The remote computer to connect to (ie. NIH Biowulf)

```
ssh user@biowulf.nih.gov
```

Users will then be asked to enter a password for signing onto Biowulf. This is the password that the user utilizes to sign onto NIH applications. The password will not appear as the user is typing but keep typing and hit enter when done.

```
user@biowulf.nih.gov's password:
```

Changing into the User's Data Folder

Upon signing onto Biowulf, users will land in the `/home/user` directory (again replace user with user's NIH username). This directory only has 16 GB of storage space and cannot be increased, thus users will need to perform analyses in the `/data/user` folder. Further, a folder called `/PartekFlow` in the `/data/user` directory is created when the Partek Flow account is activated for the user.

To check which folder on Biowulf a user is currently in, use the `pwd` command.

Upon signing onto Biowulf:

```
pwd
```

```
/home/user
```

To change into the user's `data` folder do the following.

```
cd /data/user
```

Biowulf staff will create a folder called `PartekFlow` in the user's `/data/user` directory upon activating a Partek Flow account. This folder contains all Partek Flow projects, inputs, outputs, and data Uploads.

List the contents of the `/data/user` folder.

```
ls /data/user
```

```
PartekFlow
```

Change into the `PartekFlow` folder.

```
cd /data/user/PartekFlow
```

The `PartekFlow` folder houses project folders (only if users have projects), which contain input and output as well a folder called `uploads` that stores data that has been loaded to the NIH Partek Flow server.

```
Project_RNAsequencing_1234  
uploads
```

Note

Most likely, Partek Flow users will not have to use the command line to do anything Partek Flow related as tasks such as creating projects, deleting projects, uploading files, etc. can be done in the software or using Globus.

Transferring Data to the NIH Partek Flow Server Using Globus

Globus

NCI CCR researchers will likely use the NCI CCR Sequencing Facility (or SF) (https://bioinformatics.ccr.cancer.gov/docs/resources-for-bioinformatics/raw_data_from_cores/) for sequencing projects. Data generated from the NCI CCR SF will be stored within its Data Management Environment (DME). Researchers can use Globus to transfer data from NCI CCR SF DME to the NIH Partek Flow server and the steps for accomplishing this are described below.

Note

The staff at Biowulf has created detailed documents for Globus, which can be found at <https://hpc.nih.gov/docs/globus/setup.php> (<https://hpc.nih.gov/docs/globus/setup.php>).

Step 1: Logging into Globus

Goto <https://www.globus.org> (<https://www.globus.org>) to log in by clicking on the "LOG IN" icon at the top right corner of the page.



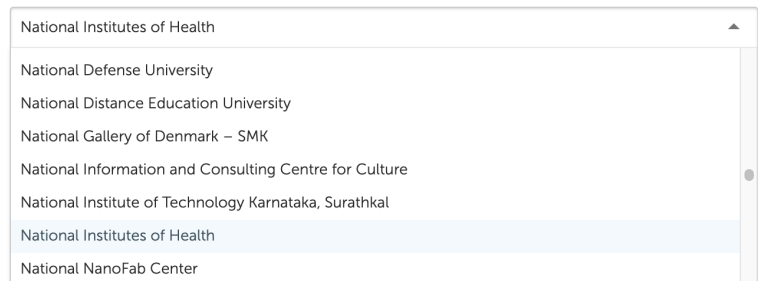
In the next page, select organizational affiliation from the drop down menu (in this example it is National Institutes of Health).



Log in to use Globus Web App

Use your existing organizational login

e.g., university, national lab, facility, project



Click on "Continue" when the organizational affiliation has been selected.



Log in to use Globus Web App

Use your existing organizational login

e.g., university, national lab, facility, project




By selecting Continue, you agree to Globus [terms of service](#) and [privacy policy](#).



Globus uses CILogon to enable you to Log In from this organization. By clicking Continue, you agree to the [CILogon privacy policy](#) and you agree to share your username, email address, and affiliation with CILogon and Globus. You also agree for CILogon to issue a certificate that allows Globus to act on your behalf.

Subsequently, users will be taken to the NIH authentication page. Click on "Sign in" to authenticate using PIV card.


 **National Institutes of Health**
Turning Discovery Into Health

Sign in

Smart Card Login

Insert your PIV card into your smart card reader or sign in using your mobile PIV-D credentials. [Need help?](#)

Sign in



Authenticator App

Use your account credentials and check your phone for a one-time code or push notification. [Need help?](#)


Username

Password

[Forgot Password?](#)

Sign in

Next, select the appropriate PIV card certificate (usually the one with the user's name followed by "- A (Affiliate)") and a pop-up will appear to take the user's NIH pin.

 **National Institute**
Turning Discovery Into Hea

Sign in

Smart Card

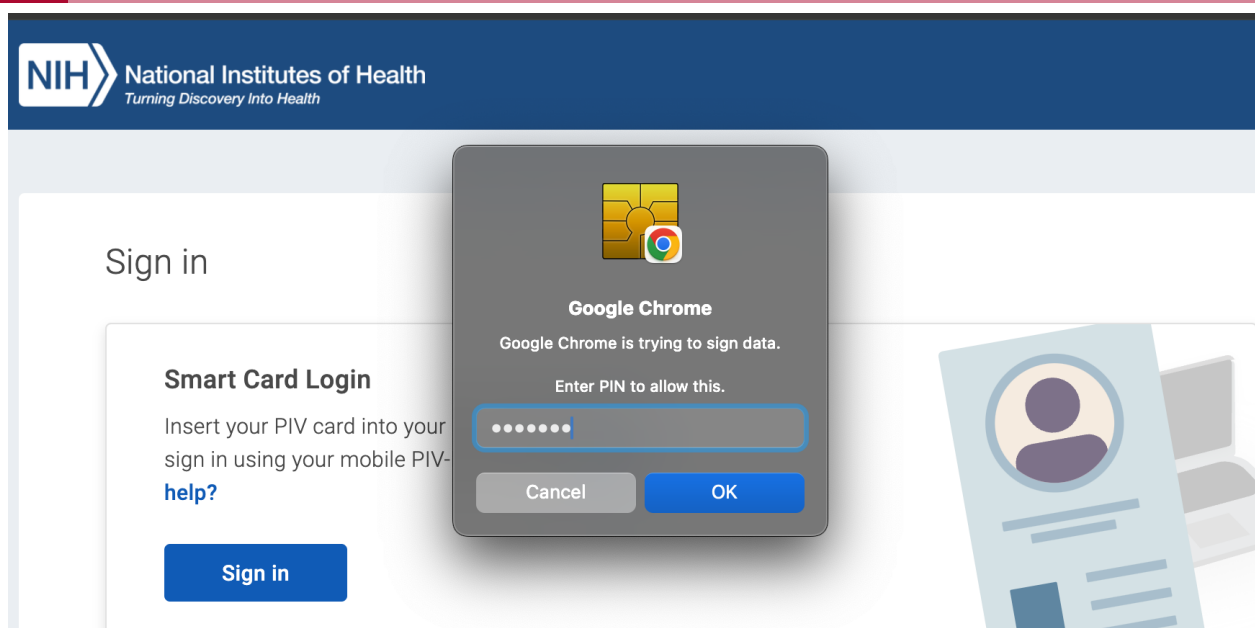
Insert your PIV

Select a certificate

Select a certificate to authenticate yourself to pivauth.nih.gov:443

Subject	Issuer	Serial
0536341A-5A96-49CA-97CA...	NIH/NCI - Rockvill...	00EAF8BE5
name -A (Affiliate)	HHS-FPKI-Interme...	61E6C307

Certificate Information **Cancel** **OK**



In the next page, scroll to the bottom and click "I Agree".



Here's the information to be released

First name: First

Last name: Last

E-mail address: First.Last@nih.gov

NetID: userid@nih.gov

The privacy policy of the service you're connecting to details things like why the service requires this information, how long the information will be retained, who the information will be shared with, etc. In general, the information is needed to facilitate your access, it will not be shared, and it will be retained for a limited time. You can review the service's privacy policy here:

<https://www.cilogon.org/privacy>



Do you agree to release the information listed above to this service?

Please select your sharing preference from the options below and click on the I Agree button.

☒ **Ask me again at next login**

- I agree to send my information this time, but I want to be prompted again the next time I access a service that requests this information.

☐ **Ask me again if information to be provided to this service changes**

- I agree to send the information listed above to this service now and in the future but I wanted to be prompted if the information the service requires changes.

☐ **Send now and in the future - Do not ask me again**

- I agree to release the information listed above to this service and to any service that asks for the same information. I want to be prompted if a service asks for different information.

I Do Not Agree

I Agree



Users will then be brought to the Globus interface where file transfers are managed. Click on "COLLECTIONS" to see the recently used Globus data transfer endpoints here. The "NIH HPC Data Transfer (Biowulf)" (<https://hpc.nih.gov/docs/globus/setup.php#endpoints>) endpoint points to the content available on the cluster.

Step 2: Setting up a Globus Endpoint to the Partek Flow Server

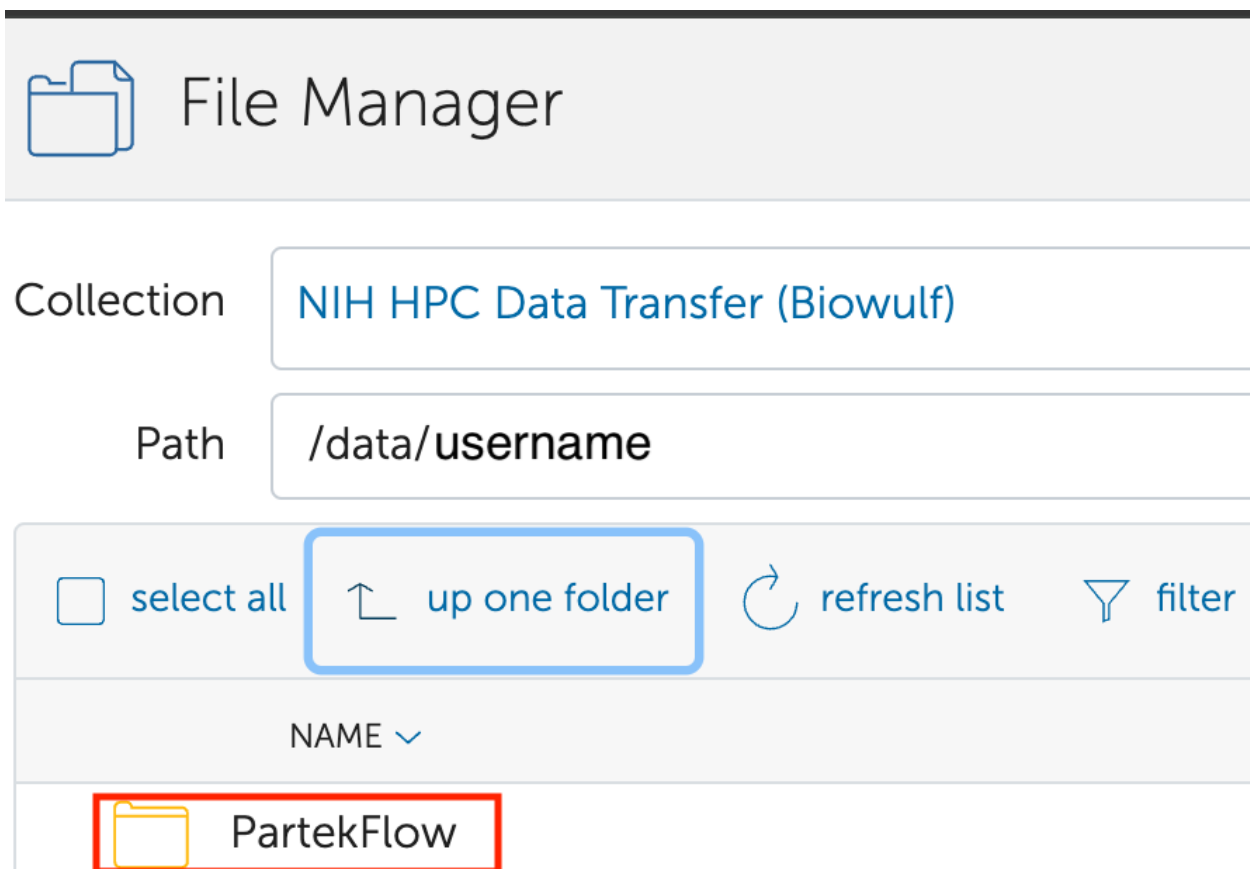
Click on the "NIH HPC Data Transfer (Biowulf)" endpoint and then "Open in File Manager". This will take users to their Biowulf /home directory. Username is the Biowulf user name for the specific user.

Recall

The user's Biowulf /home directory is not suitable for analyzing data. To conduct analysis, use the /data directory.

To goto the user's /data/directory, replace /home/username in the box labeled "Path" with /data/username.

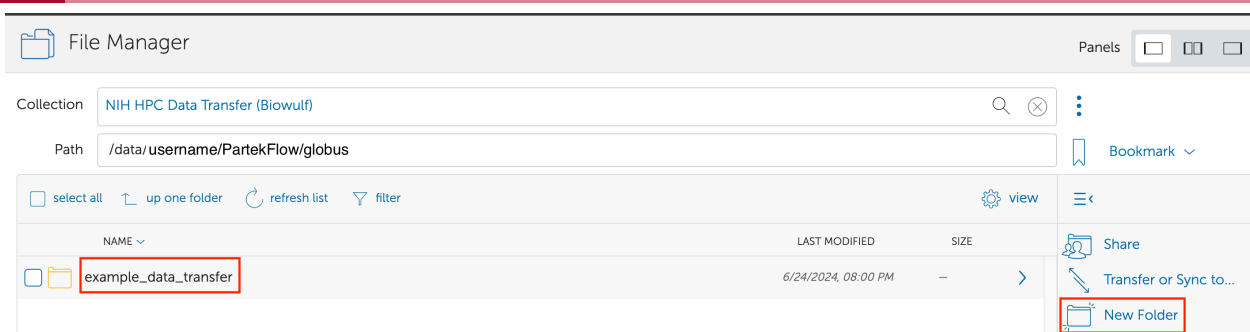
After switching to the user specific `/data` directory, find and click into the **PartekFlow** folder. Recall that the **PartekFlow** folder will exist only if the user has contacted Biowulf staff about activating a Partek Flow account.



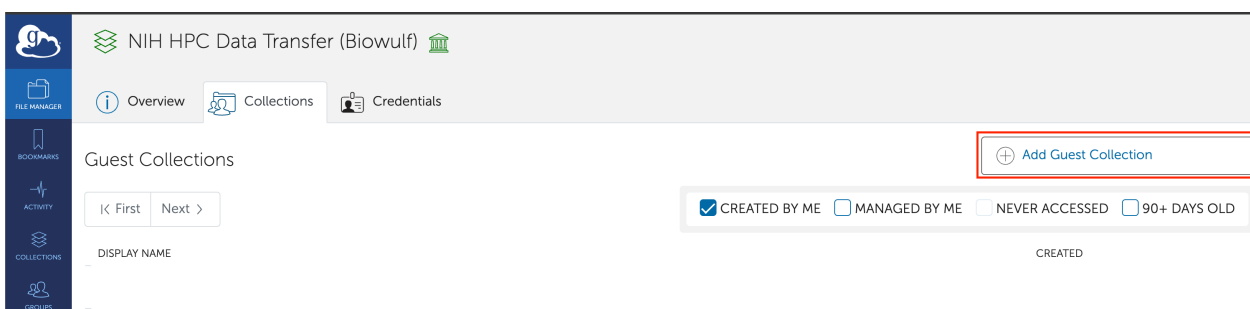
Next, click on "New Folder" to make a folder called "globus" to store data uploaded to the Partek Flow server via Globus.




Then, click into the `globus` folder and create one named `example_data_transfer`.



Go back to the "NIH HPC Data Transfer (Biowulf)" endpoint and click on the "COLLECTIONS" tab after the `example_data_transfer` folder has been created. From there, click on "Add Guest Collection".



In the "Add Guest Collection" menu, click "Browse" to select the folder in which the endpoint will reference (ie. `/data/username/PartekFlow/globus/example_data_transfer`). Enter a display name and description for the endpoint and then "Create Collection" when ready.



Create new Guest Collection

You are creating a guest collection on **NIH HPC Data Transfer (Biowulf)** to share data

Directory ✓ Browse ?

↑ up one folder
↻ refresh list
☰

This folder is empty.

Display Name

Description


Keywords

☐ Force encryption on transfers to and from this collection

[view more fields](#) ▼

Create Collection
Cancel

The user will then be taken to a page for setting up sharing between the endpoint and the location where the data is (ie. NCI CCR Sequencing Facility DME).



example data transfer

Overview
Permissions
Roles

Shared With


Mapped Collection: NIH HPC Data Transfer (Biowulf)
Base Path: /data/wuz8/PartekFlow/globus/example_data_transfer/

USER OR GROUP
CREATED
EXPIRATION
READ
WRITE


▼
Permissions granted by role

Add Permissions — Share With

Leave the entry in the box labeled "Path" as "/". Make sure to mark the "Write" permission box because the NCI CCR Sequencing Facility DME has to write the data into this Globus endpoint. Then click "Select a Group" to choose the group in which to share /data/username/PartekFlow/globus/example_data_transfer with.

 EXAMPLE DATA TRANSFER

Add Permissions - Share With

Path  [Browse](#)

Share With

- ☐ user - share with specific individuals
- ☒ group - make data accessible to members of a group
- ☐ all users - make data accessible to all logged in users of Globus
- ☐ public (anonymous) - make data accessible to everyone


Group [Select a Group](#)

Permissions

- ☒ read
- ☒ write


[Add Permission](#) [Cancel](#)

In the drop down menu, select "HPCDME-PROD-App-Accts-Pool-FNLCR" to return to the "Add Permissions" page. Hit "Add Permission" when ready.

 EXAMPLE DATA TRANSFER

Select a Group

Search by group name or select one below



- HPCDME-PROD-App-Accts-Pool-CCBR
- HPCDME-PROD-App-Accts-Pool-HITIF
Pool of Globus app accounts for the NIH NCI DOC known as HiTIF
- HPCDME-DEV-App-Accts-Pool-FNLCR
HPC DME Globus Group for FNLCR
- HPCDME-PROD-App-Accts-Pool-FNLCR**
Pool of Globus app accounts for the NIH NCI DOC of the Sequencing Facility at FNLCR

Click "Done" to finish the adding permission process.

EXAMPLE DATA TRANSFER
Add Permissions - Share With

Path: ✓ Browse

Share With:

- ☐ user - share with specific individuals
- ☒ group - make data accessible to members of a group
- ☐ all users - make data accessible to all logged in users of Globus
- ☐ public (anonymous) - make data accessible to everyone

Group: Change

Permissions:

- ☒ read
- ☒ write

Add Permission

Permissions Added

Read and write permissions were added for HPCDME-PROD-App-Accts-Pool-FNLCR on path: /

Add another Permission Done

The user will then be returned to the "example data transfer" endpoint and see that this endpoint has been shared with "HPCDME-PROD-App-Accts-Pool-FNLCR".

example data transfer

Overview Permissions Roles

Shared With Add Permissions — Share With

Mapped Collection: NIH HPC Data Transfer (Biowulf)
Base Path: /data/wuz8/PartekFlow/globus/example_data_transfer/

USER OR GROUP	CREATED	EXPIRATION	READ	WRITE
<div>Permissions granted by role</div> <div> <div>Path: /</div> <div>Show link for sharing</div> </div>				
HPCDME-PROD-App-Accts-Pool-FNLCR	6/24/2024, 09:34 PM	never expires	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Click on the "Overview" tab and scroll to the bottom of the page. Take note of the UUID, which tells Sequencing Facility DME where to send data. The UUID for each Globus endpoint will be different.

example data transfer

Overview Permissions Roles

User Message	(not set)
User Message Link	(not set)
Information Link	(not set)
Contact Email	(not set)
Organization	(not set)
Department	(not set)
Other Contact Info	(not set)
Visible To	Public - Visible to all users
Force Encryption	No
Subscription	NIH Helix Systems
Multi-factor authentication required	No
UUID	db2c77a9-4134-47bf-b4f3-25e3bb6a24cb

Step 3: Downloading Data from the NCI CCR SF DME

Copy the link to the data provided by the NCI CCR SF and sign in with user specific NIH credentials and the page below will be shown. Users can download all data or browse through their data.

NIH NATIONAL CANCER INSTITUTE

Data Management Environment

Joe Wu Help version: 3.2.1

Dashboard Register Search Browse Manage

Collection

Download all data Browse project data

Path: /FNL_SF_Archive/PI_Lab_SF_Lab/Project_SF_RnD_CS026880_4scRNAseq_030620

Parent Name: /FNL_SF_Archive/PI_Lab_SF_Lab

Collection Size: 49844727842 (49.8 GB)

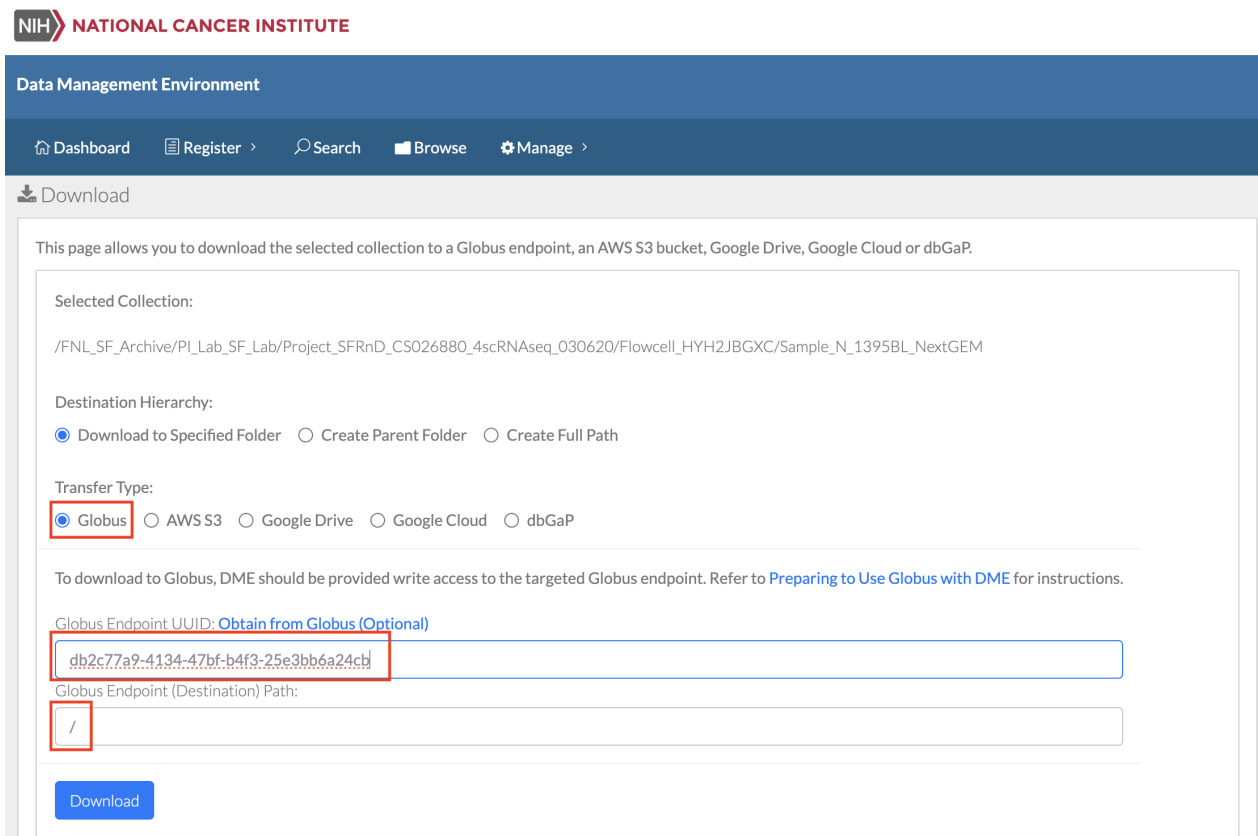
User Metadata

Attribute Name
bioinformatics_contact
contact_name
grant_funding_agent
project_id_CSAS_NAS
project_name
project_start_date
project_status
retention_years

This example will click on the tab for browsing data and download FASTQ files in the folder labeled "Sample_N_1395BL_NextGEM". To download, just click on the "down arrow" corresponding to this folder in the column labeled "Download".



After clicking on the download arrow, users will be taken to the dialogue page shown below. Be sure to select Globus for the "Transfer Type", go back to Globus and copy then paste the endpoint UUID (this will ensure that the data gets transferred to the right place), and finally, leave the path as "/" as it was set when creating the "example data transfer" Globus Endpoint. When ready, hit "Download".



If all goes well, users will see a message indicating that the data transfer request has been submitted successfully.

Data Management Environment

[Dashboard](#) [Register >](#) [Search](#) [Browse](#) [Manage >](#)

Download

This page allows you to download the selected collection to a Globus endpoint, an AWS S3 bucket, Google Drive, Google Cloud or dbGaP.

Selected Collection:

/FNL_SF_Archive/PI_Lab_SF_Lab/Project_SFRnD_CS026880_4scRNAseq_030620/Flowcell_HYH2JBGXC/Sample_N_1395BL_NextGEM

Destination Hierarchy:

☒ Download to Specified Folder ☐ Create Parent Folder ☐ Create Full Path

Asynchronous download request is submitted successfully! Task Id: 899e5011-06ef-46ef-a3e4-6b644e0f3c3e

Click on "Manage" and then "Download Tasks" to check download progress. Each download is assigned a task ID.

Data Management Environment

[Joe Wu](#) [Help](#) version: 3.2.1

[Dashboard](#) [Register >](#) [Search](#) [Browse](#) [Manage >](#)

Download Tasks

My Tasks

[Notifications](#)
[Download Tasks](#)
[Registration Tasks](#)

Current page 1 of 1 | Page Size: 47 | Total Records: 47

[First](#) [Previous](#) [Next](#) [Last](#)

Task ID	Path	Type	Destination Type	Created On	Completed On	Transfer Result	Retry User ID	Error
Filter by Task ID	Filter by Path	Filter by Type	Filter by Destination	Filter by Created	Filter by Completed	Filter by	Filter by Ret	Filter by Error
899e5011-06ef-46ef-a3e4-6b644e0f3c3e	/FNL_SF_Archive/PI_Lab_SF_L...	COLLECTION	GLOBUS	06/25/2024 11:42		In Process		

Go back to the "example data transfer" endpoint on Globus and click on "Open in File Manager".

example data transfer

[FILE MANAGER](#)
[OVERVIEW](#)
[Permissions](#)
[Roles](#)

Display Name example data transfer

Entity Type Guest Collection (GCS)

Mapped Collection NIH HPC Data Transfer (Biowulf)

Endpoint NIH HPC Data Transfer

Last Accessed 2024-06-25T00:00:00+00:00

Domain g-9982898.8c9063.a567.data.globus.org

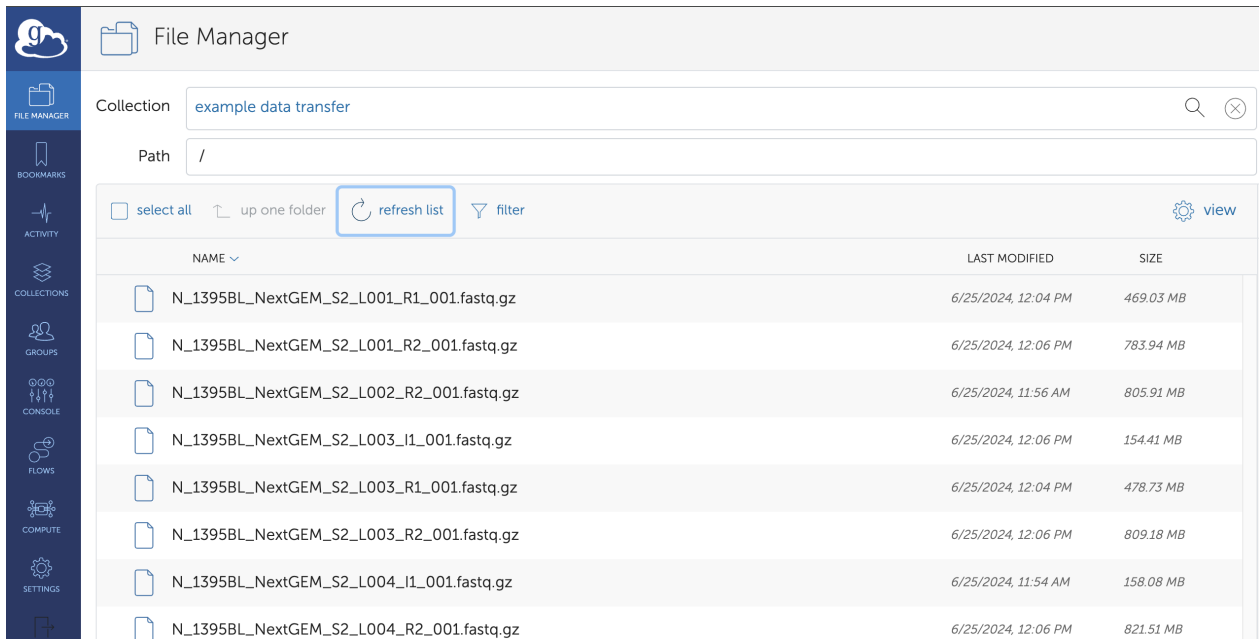
Advertised Owner wuz8@nih.gov

Original Owner NIH HPC Prod V5 (00734248-ac2a-4e65-bbb0-23ea6818d5ff@clients.auth.globus.org)

Description Endpoint for transferring data from the NCI CCR Sequencing Facility Data Management Environment to the NIH Partek Flow server.

[Manage Consent](#)
[Edit Attributes](#)
[Open in File Manager](#)
[View Collection Activity](#)
[Delete Collection](#)

The data will populate in the `data/username/PartekFlow/globus/example_data_transfer` folder (ie. the folder pointed to by the "example data transfer" endpoint) as the download proceeds.



The screenshot shows the File Manager interface. The 'Collection' field is set to 'example data transfer'. The 'Path' is '/'. The 'refresh list' button is highlighted with a blue box. The table below lists the files in the collection.

NAME	LAST MODIFIED	SIZE
N_1395BL_NextGEM_S2_L001_R1_001.fastq.gz	6/25/2024, 12:04 PM	469.03 MB
N_1395BL_NextGEM_S2_L001_R2_001.fastq.gz	6/25/2024, 12:06 PM	783.94 MB
N_1395BL_NextGEM_S2_L002_R2_001.fastq.gz	6/25/2024, 11:56 AM	805.91 MB
N_1395BL_NextGEM_S2_L003_I1_001.fastq.gz	6/25/2024, 12:06 PM	154.41 MB
N_1395BL_NextGEM_S2_L003_R1_001.fastq.gz	6/25/2024, 12:04 PM	478.73 MB
N_1395BL_NextGEM_S2_L003_R2_001.fastq.gz	6/25/2024, 12:06 PM	809.18 MB
N_1395BL_NextGEM_S2_L004_I1_001.fastq.gz	6/25/2024, 11:54 AM	158.08 MB
N_1395BL_NextGEM_S2_L004_R2_001.fastq.gz	6/25/2024, 12:06 PM	821.51 MB

These changes are also reflected on Biowulf. Again, replace username with the user's Biowulf user name.

```
ls /data/username/PartekFlow/globus/example_data_transfer
```

```
N_1395BL_NextGEM_S2_L001_I1_001.fastq.gz
N_1395BL_NextGEM_S2_L001_R1_001.fastq.gz
N_1395BL_NextGEM_S2_L001_R2_001.fastq.gz
N_1395BL_NextGEM_S2_L002_I1_001.fastq.gz
N_1395BL_NextGEM_S2_L002_R1_001.fastq.gz
N_1395BL_NextGEM_S2_L002_R2_001.fastq.gz
N_1395BL_NextGEM_S2_L003_I1_001.fastq.gz
N_1395BL_NextGEM_S2_L003_R1_001.fastq.gz
N_1395BL_NextGEM_S2_L003_R2_001.fastq.gz
N_1395BL_NextGEM_S2_L004_I1_001.fastq.gz
N_1395BL_NextGEM_S2_L004_R1_001.fastq.gz
N_1395BL_NextGEM_S2_L004_R2_001.fastq.gz
```

Transferring Data to the NIH Partek Flow Server Using Command Line

Note

Command line uploads can be used when the files are already present on Biowulf. -- Biowulf (https://partekflow.cit.nih.gov/#upload_commandline)

Copy from User's Biowulf data Folder to Partek Flow uploads Folder

Copying from user's Biowulf /data directory to the uploads subfolder in PartekFlow is allowed. Be sure to be in an interactive session for this by using the `sinteractive` command. For instance:

To transfer the folder `hbr_uhr_fastq_download` in `/data/username` to the uploads subfolder in PartekFlow, do the following. Replace username with the user's Biowulf user name.

```
cp -r /data/username/hbr_uhr_fastq_download /data/username/PartekFlow/uploads
```

Note that the Biowulf user owns the `hbr_uhr_fastq_download` PartekFlow. This enables users to delete the folder. The `ls` command lists directory content and the `-l` option list the content in long or detailed format.

```
[wuz8@cn4304 username]$ ls -l /data/username/PartekFlow/uploads/  
drwxr-s---+ 2 username      partekfl 4096 May 28 11:55 hbr_uhr_fastq_download
```

It is possible to change into the upload subfolder in `/data/username/PartekFlow` and make a directory using the `mkdir` command.

```
cd /data/username/PartekFlow/uploads
```

```
[username@cn4304 uploads]$ mkdir hbr_uhr_fastq
```

Again the user owns the directory, and thus can delete it. Creating folders is a good way to keep data organized for analyses.

```
[wuz8@cn4304 uploads]$ ls -l
drwxrws---+ 2 username      partekfl 4096 May 28 13:12 hbr_uhr_fastq
```

Tip

File transfer using command line:

- Copy from data folder to Partek Flow uploads folder is **OK**
- Copy from data folder to Partek Flow directory is **OK**
- Copy from data folder to Partek Flow project folder is **not OK**
- Copy from Partek Flow uploads folder to project folder is **not OK**

Caution

While the above command line methods for data transfer are valid, users should remember that: "Virtually all file transfer activities should be run from within the web interface, rather than from the command line. We have implemented a permissions policy on users' PartekFlow directories to prevent inadvertent file removal mistakes that breaks the old way of moving files around." -- Biowulf staff

scp from Personal Computer to the Partek Flow uploads Folder.

The scp commands enables users to securely transfer data to and from personal computer to a remote computer such as a high performance computing system. To transfer data from personal computer to the Partek Flow uploads folder do the following.

Note

Helix is the node on the Biowulf system that is intended for data transfer.

```
scp local_file username@helix.nih.gov:/data/username/PartekFlow/uploa
```

Enter user's Biowulf password.

For example, the following command construct will transfer the folder hbr_uhr_fastq on local computer that contains FASTQ files to the Partek Flow uploads folder on Biowulf. The -r option in scp will copy a folder and its content.

```
scp -r hbr_uhr_fastq_files username@helix.nih.gov:/data/username/Parte
```

```
ls -l /data/username/PartekFlow/uploads
```

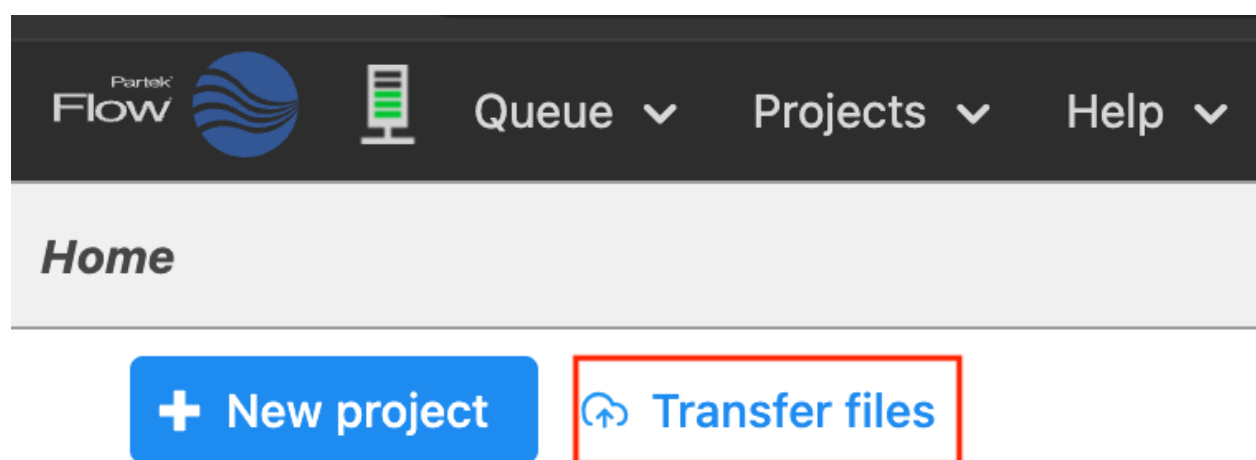
Again, the Biowulf account user owns the directory and can modify and delete it.

```
drwxr-s---+ 2 username partekfl 4096 Jun 25 21:13 hbr_uhr_fastq_files
```

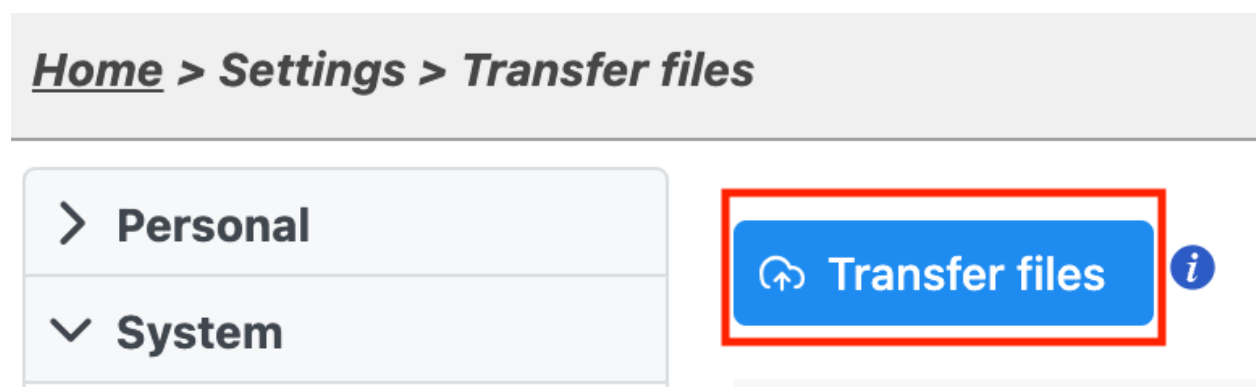
Transferring Data to the NIH Partek Flow Server Using the Web Tool

Using the Partek Flow web tool to transfer data

If users have data stored on a personal computer, the Partek Flow web tool can be used to transfer data onto the server. Upon signing in to Partek Flow, a button labeled "Transfer files" is available. Click on this.



This takes the users to the "Transfer files" section of the settings page. Click on the blue "Transfer files" tab at the top.

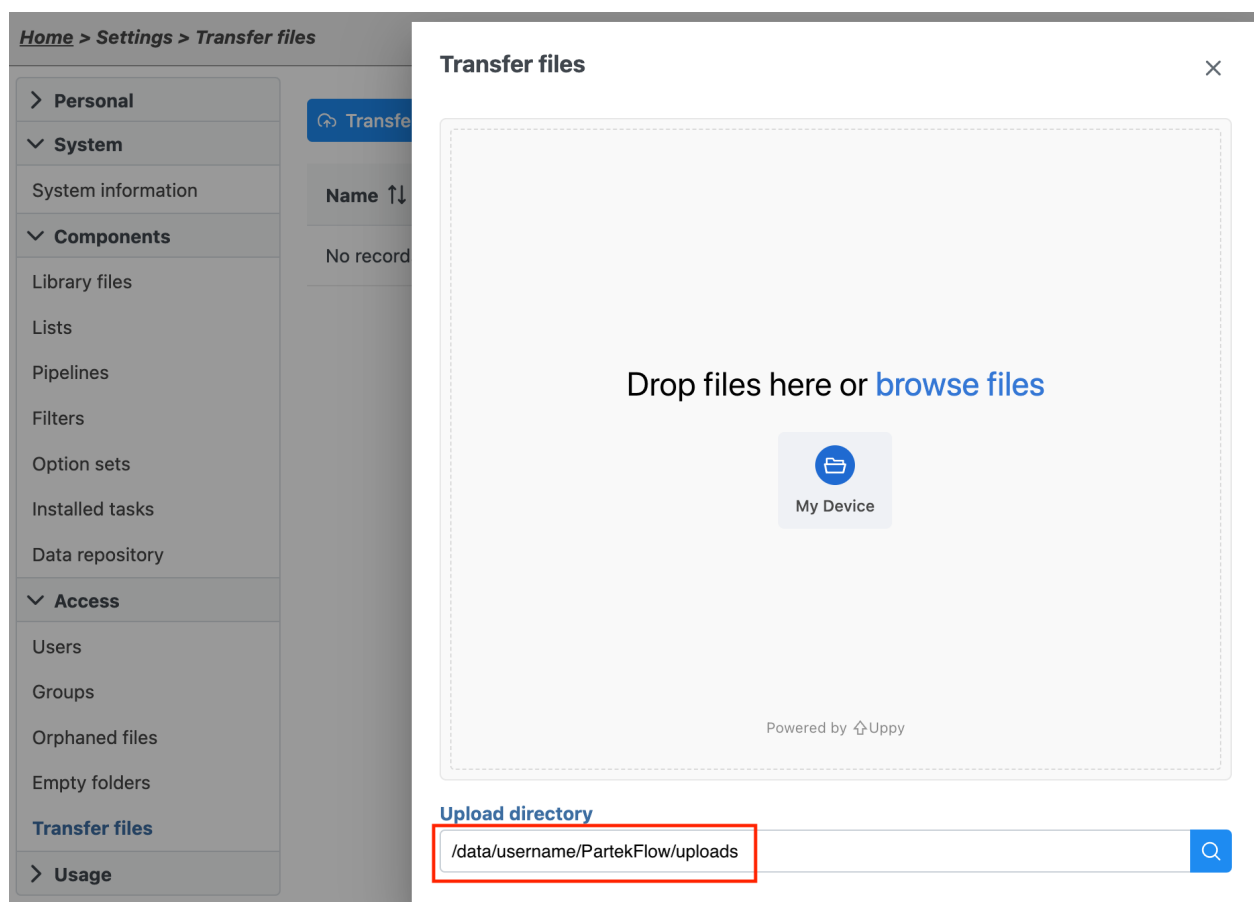


A dialogue box that assists the user with data transfer appears.

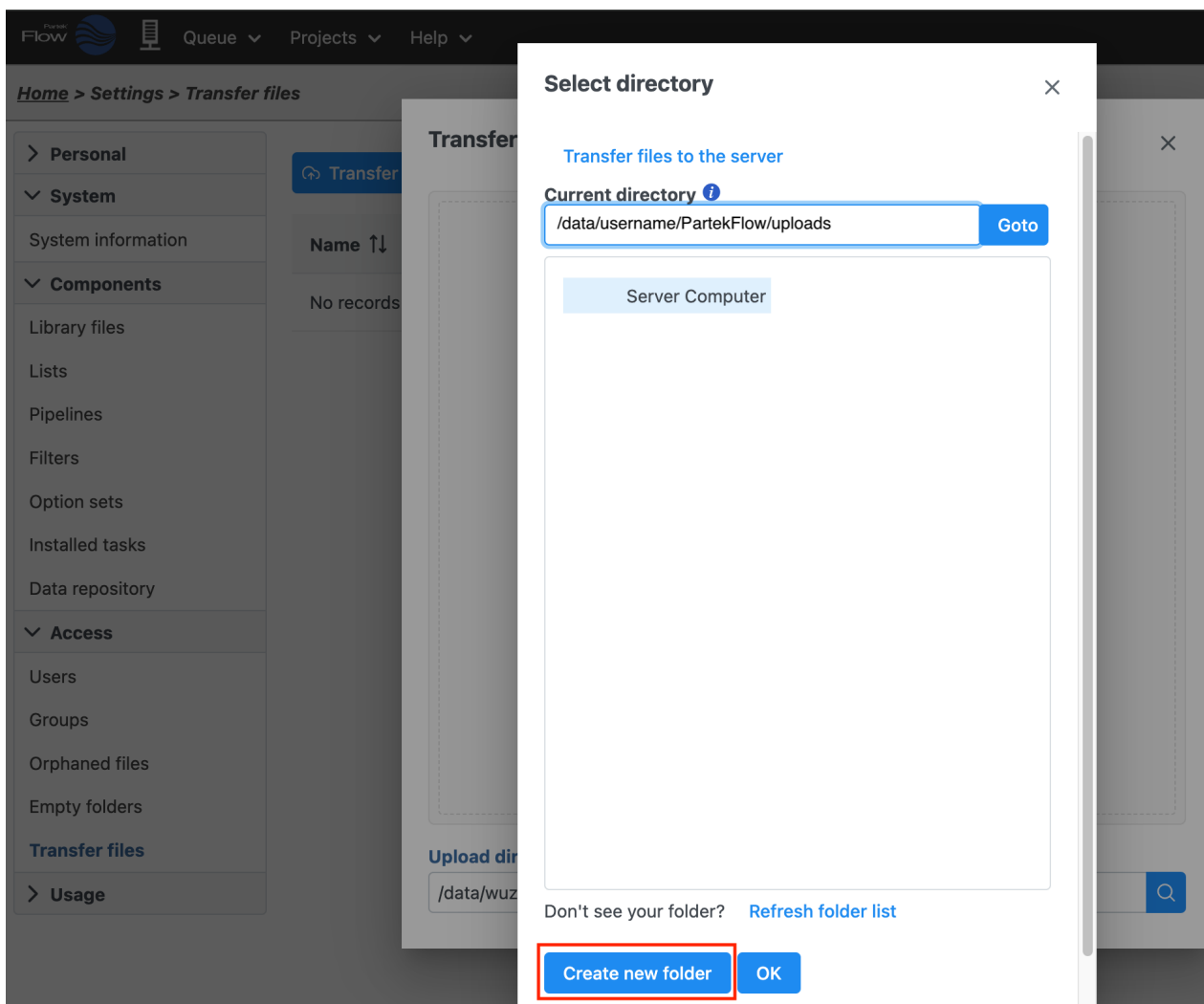
Note

Users can only transfer to the Partek Flow uploads folder or subfolders within uploads.

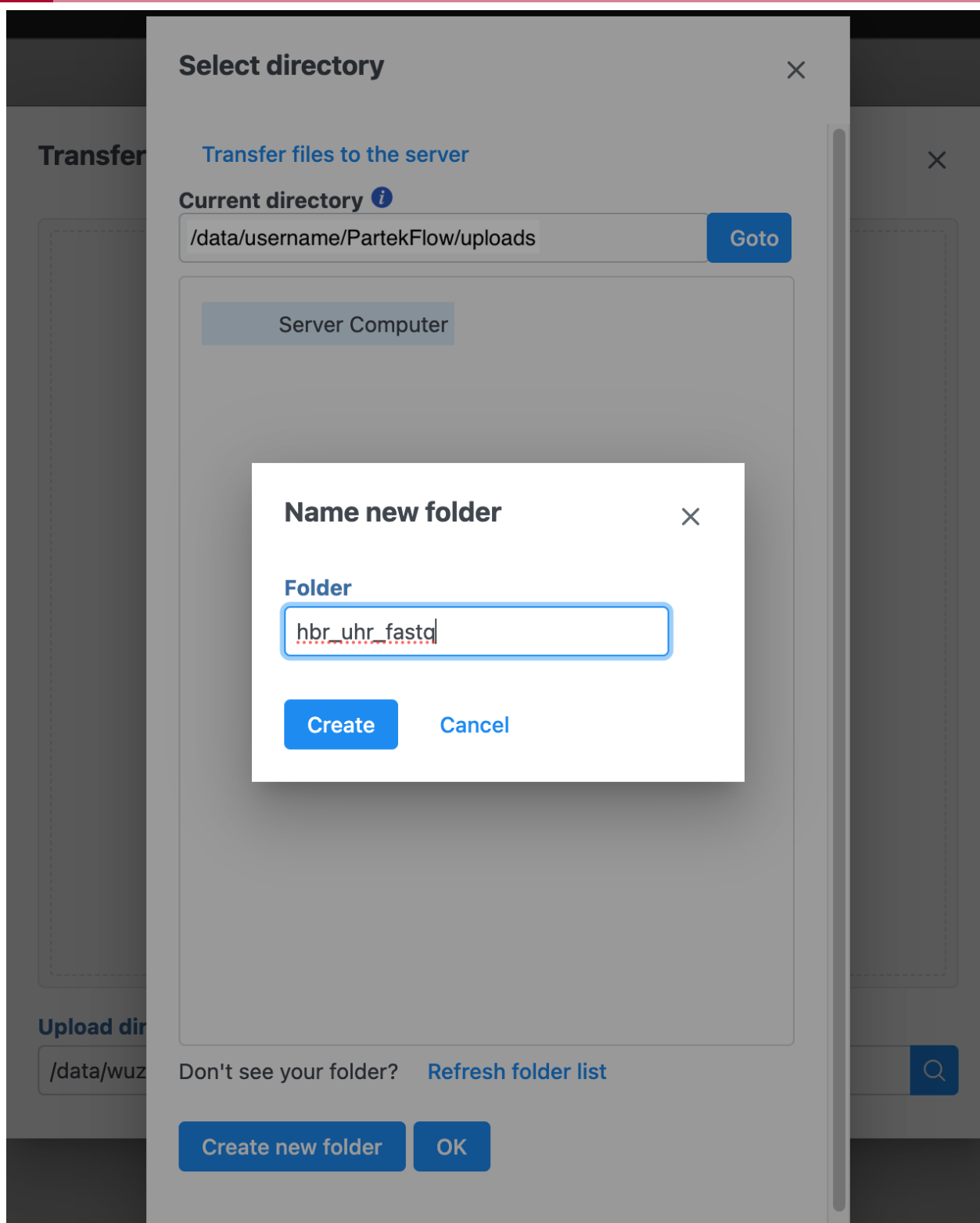
The current "Upload directory" as indicated at the bottom of the file transfer dialogue box is /data/username/PartekFlow/uploads. Click on the magnifying glass next to it to create new folders within Partek Flow uploads to store data uploaded for specific projects. It is a good idea to create a folder to store data for each project.



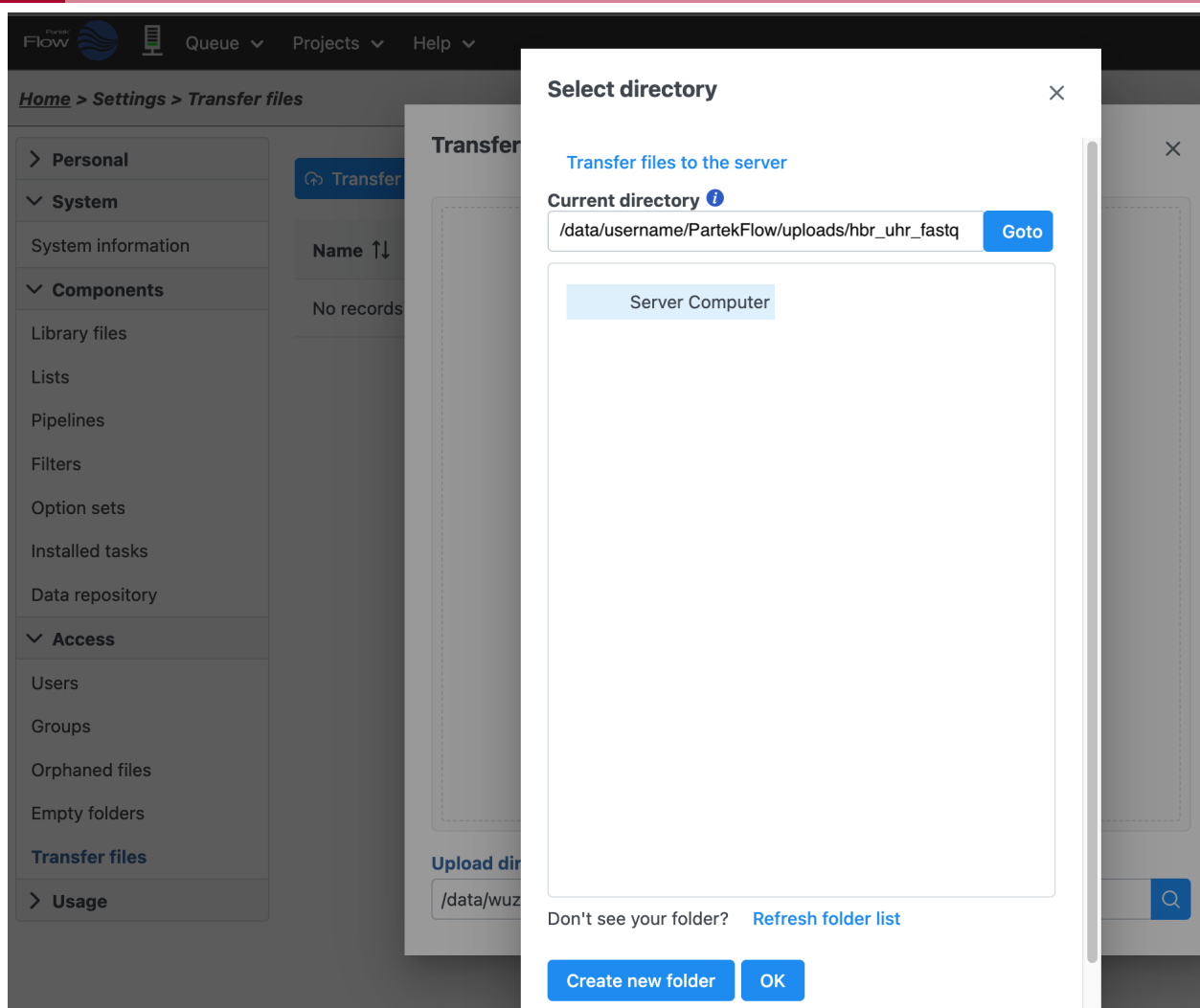
To create a new folder, click on the blue "Create new folder" tab.



Enter the name of the folder (ie. hbr_uhr_fastq) and click the blue "Create" tab when ready.



The "Current directory" is updated to reflect that the user is now in /data/username/PartekFlow/uploads/hbr_uhr_fastq.





Click "Ok" to return to the file transfer dialogue box. Note that the "Upload directory" has been updated to /data/username/PartekFlow/uploads/hbr_uhr_fastq as well.


Twelve FASTQ files will be transferred to the folder hbr_uhr_fastq in uploads. Users can either drag and drop or browse to select files for upload. Click the green "Upload" button when ready (the number shown inside this button depends on the number of items to be transferred).




Transfer files

[Cancel](#)12 files selected[+ Add more](#)


UHR_1_R1.fq
53 MB


HBR_1_R2.fq
28 MB

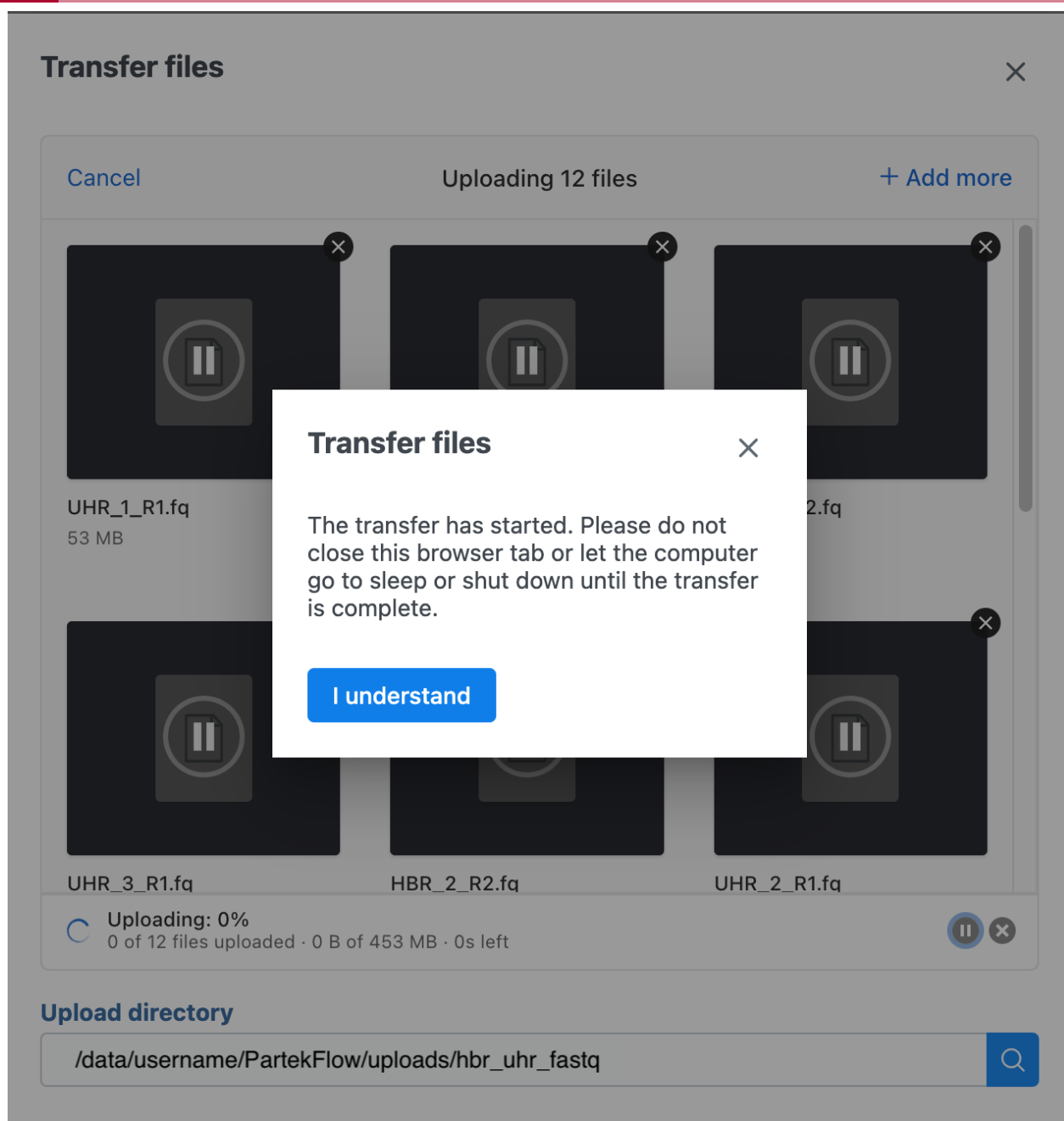

HBR_3_R2.fq
30 MB

[Upload 12 files](#)

Upload directory

The warning message below will appear once the data transfer has commenced. Click "I understand".



A bar indicating the transfer status will also appear.

Transfer files



Cancel
Uploading 10 files
+ Add more

UHR_1_R1.fq
53 MB

HBR_1_R2.fq
28 MB

HBR_3_R2.fq
30 MB

UHR_3_R1.fq

HBR_2_R2.fq

UHR_2_R1.fq

Uploading: 28%
2 of 12 files uploaded · 126 MB of 453 MB · 11m 40s left

Upload directory

After the transfer is complete, users can click on the arrow next to the `/data/username/PartekFlow/upload` folder to view its subfolders and contents of subfolders.

Note

The user will not own contents transferred via the web tool. Thus, the only way to delete is using the "trash can" under the "Action" column. If user attempts to delete via command line, the message "Permission denied" will appear.

Home > Settings > Transfer files

Transfer files ⓘ

Click to hide folder content

Name ↑↓	Creator ↑↓	Size ↑↓	Last modified ↑↓	Status ↑↓	Actions
✓ /data/username/PartekFlow/uploads/hbr_uhr_fastq		453.43 MB	-	-	Delete folder
HBR_3_R1.fq	username	30.38 MB	26 Jun 2024, 02:24 PM EDT	Complete	Delete individual files
UHR_2_R1.fq	username	38.01 MB	26 Jun 2024, 02:24 PM EDT	Complete	
UHR_1_R2.fq	username	53.24 MB	26 Jun 2024, 02:24 PM EDT	Complete	

Listing the contents of the `/data/username/PartekFlow/uploads` folder on Biowulf will reveal the `hbr_uhr_fastq` subdirectory.

```
[wuz8@cn4304 username]$ ls -l /data/username/PartekFlow/uploads/
drwxrws---+ 2 partekfl partekfl 4096 May 28 14:26 hbr_uhr_fastq
```

An attempt to remove the `hbr_uhr_folder` will result in a message saying "Permission denied". In the `rm` command below, `-r` tells `rm` to remove a folder and `f` forces `rm` to delete without asking for confirmation.

```
[wuz8@cn4304 username]$ rm -rf /data/username/PartekFlow/uploads/hbr_
rm: cannot remove '/data/username/PartekFlow/uploads/hbr_uhr_fastq/hl
```

Importing Data to the Partek Flow Projects

Data import into Partek Flow projects

After data has been transferred to the NIH Partek Flow server, the next step is to import them into a project. Sign onto Partek Flow and hit the "New project" button click to create a new project called project1. The project will then appear in the project table. Click on project1 to enter the analysis interface.

Home

[+ New project](#) [Transfer files](#) Repository s

Optional columns [Q](#)


Project name ↑↓	Owner ↑↓	Your role ↑↓	Last modified ↓↑	Size ↑↓	Actions
> project1	username	Project owner	27 May 2024, 08:23 PM	0 B	⋮

Click on the round button labeled "Add data" to begin adding data to the project.

Partek Flow Queue ▾ Projects ▾ Help ▾

Home > project1 (Project owner)

[Analyses](#) Metadata Log Project settings Notebook Data viewer Attachments



Welcome to your project.

You'll need samples before you can run an analysis.
Click the blue button on the left then choose your assay and file type.

For more help please watch this [video](#) or see our [documentation](#).

Users will be greeted with a range of options for data import. In this example, click "Bulk" and then select "RNA-Seq". FASTQ files will be imported. Click "Next" when ready.

Partek Flow Queue Projects Help

Home > project1 > Initial import

Single cell **Bulk** Microarray Other

RNA-Seq ChIP/ATAC-Seq DNA-Seq Metagenomics Proteomics

Select the format

☒ **fastq**
Import unaligned reads. Acceptable file types are fastq, fastq.gz, fastq.bz2, fq, fq.gz, fq.bz2

☐ **bam**
Import aligned reads. Acceptable file types are bam, sam, and ubam

☐ **Generic Count matrix**
Import quantified data (e.g. gene counts per sample). Acceptable file types are txt, csv, tsv, txt.gz, csv.gz, tsv.gz

Back Next

In the subsequent page, the current directory is displayed in the file menu on the left.

Note

Users will only be able to access content in the `/data/username/PartekFlow` folder once signed on. So make sure to put the data there using one of the methods described in this tutorial.

This example imports the FASTQ file in `uploads/hbr_uhr_fastq`. Be sure to check the box (labeled "Name") to select all files.

Partek Flow Queue Projects Help username

Home > project1 > Initial import > Import sample files > fastq

File select

☒ Partek Flow Server ☐ URL ☐ GEO / ENA

[Transfer files to the server](#)

Current directory [i](#)
`/data/username/PartekFlow/uploads/hbr_uhr_fastq` [Goto](#)

12 files selected

<input checked="" type="checkbox"/>	Name	Size
<input checked="" type="checkbox"/>	HBR_1_R1.fq	27.76 MB
<input checked="" type="checkbox"/>	HBR_1_R2.fq	27.76 MB
<input checked="" type="checkbox"/>	HBR_2_R1.fq	33.91 MB
<input checked="" type="checkbox"/>	HBR_2_R2.fq	33.91 MB
<input checked="" type="checkbox"/>	HBR_3_R1.fq	30.38 MB
<input checked="" type="checkbox"/>	HBR_3_R2.fq	30.38 MB
<input checked="" type="checkbox"/>	UHR_1_R1.fq	53.24 MB
<input checked="" type="checkbox"/>	UHR_1_R2.fq	53.24 MB
<input checked="" type="checkbox"/>	UHR_2_R1.fq	38.01 MB
<input checked="" type="checkbox"/>	UHR_2_R2.fq	38.01 MB

Don't see your folder? [Refresh folder list](#)

Valid files are: fastq

Scroll to the bottom of the data import page and select the data type (ie. mRNA) and click "Finish".

File select

☒ Partek Flow Server ☐ URL ☐ GEO / ENA

[Transfer files to the server](#)

Current directory [Goto](#)

/data/username/PartekFlow/uploads/hbr_uhr_fastq

12 files selected

Name	Size
<input checked="" type="checkbox"/> HBR_1_R1.fq	27.76 MB
<input checked="" type="checkbox"/> HBR_1_R2.fq	27.76 MB
<input checked="" type="checkbox"/> HBR_2_R1.fq	33.91 MB
<input checked="" type="checkbox"/> HBR_2_R2.fq	33.91 MB
<input checked="" type="checkbox"/> HBR_3_R1.fq	30.38 MB
<input checked="" type="checkbox"/> HBR_3_R2.fq	30.38 MB
<input checked="" type="checkbox"/> UHR_1_R1.fq	53.24 MB
<input checked="" type="checkbox"/> UHR_1_R2.fq	53.24 MB
<input checked="" type="checkbox"/> UHR_2_R1.fq	38.01 MB
<input checked="" type="checkbox"/> UHR_2_R2.fq	38.01 MB

Don't see your folder? [Refresh folder list](#) Valid files are: fastq

☒ **Select data type: (only required for multi assay project)**

If none of the preset options matches your data, choose custom and add a custom type.

mRNA

[Back](#) [Finish](#)

A rectangle labeled "Importing" will appear as data is being imported into a project.

Partek Flow Queue Projects Help

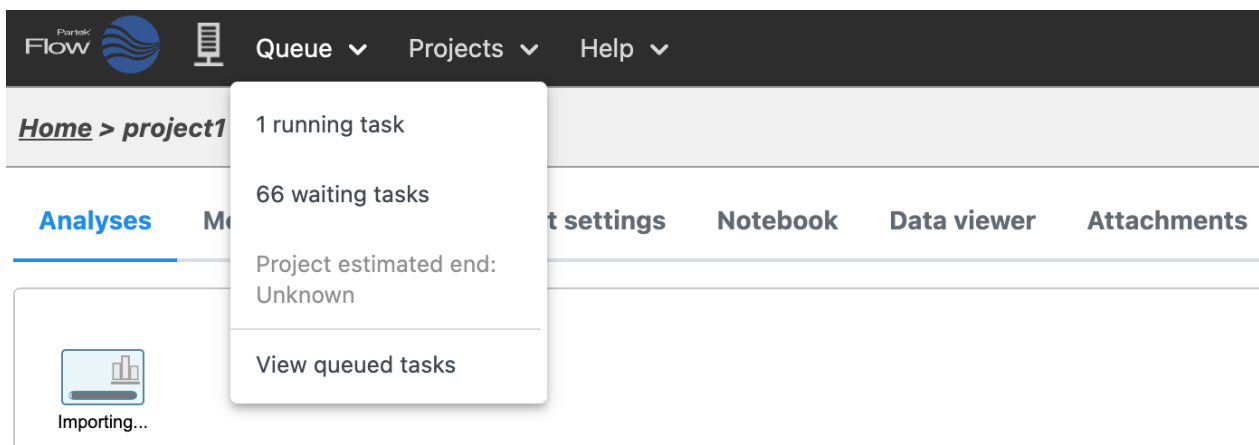
Home > project1 (Project owner)

Analyses Metadata Log Project settings Notebook Data viewer Attachments

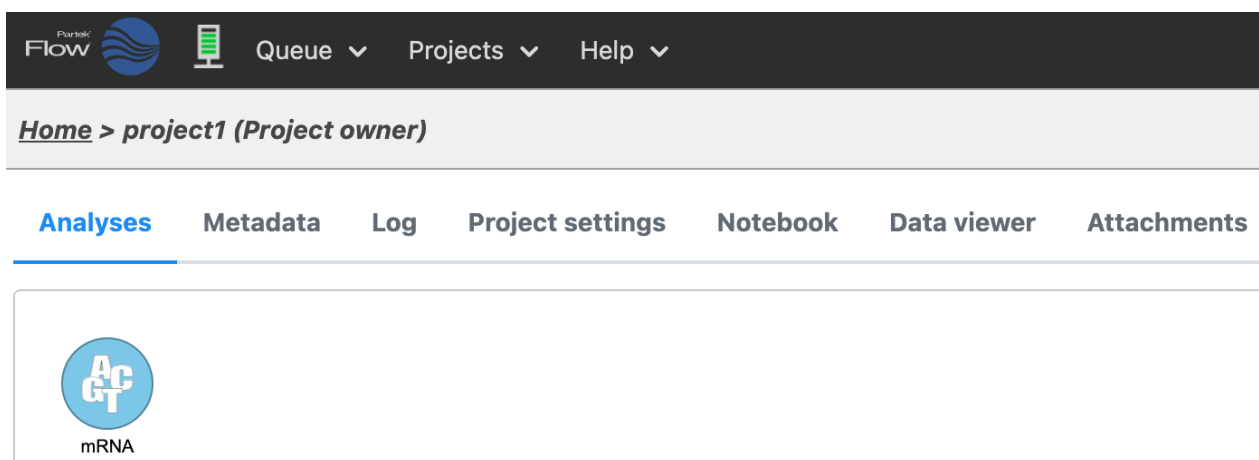
Importing...

Tip

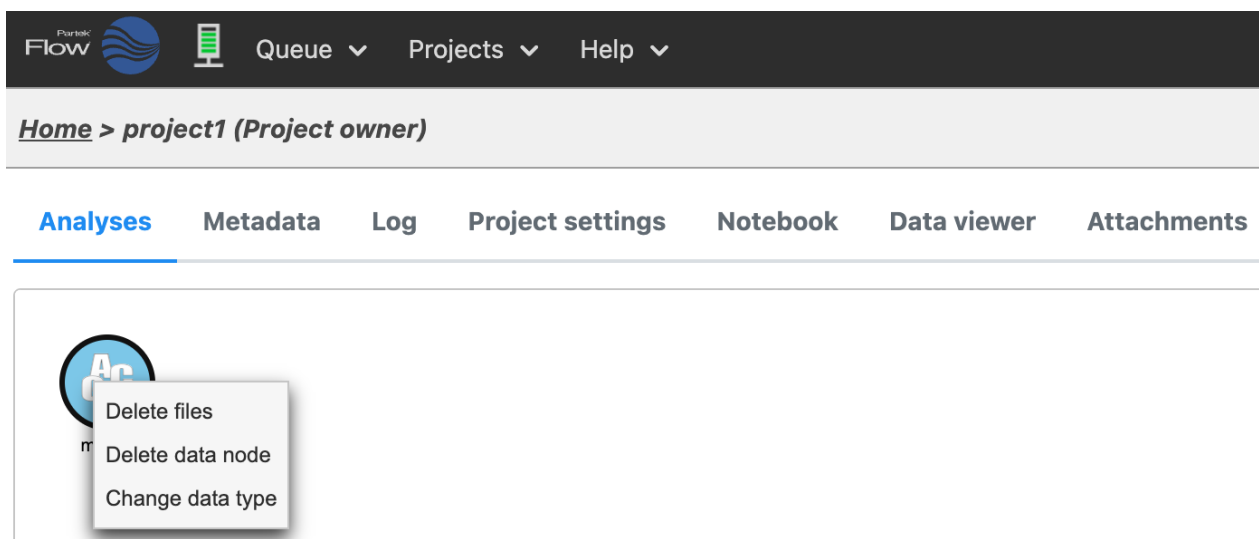
The time it takes to import or to complete a task in Partek Flow depends on the queue. If the queue is long, then it's time for a coffee break.



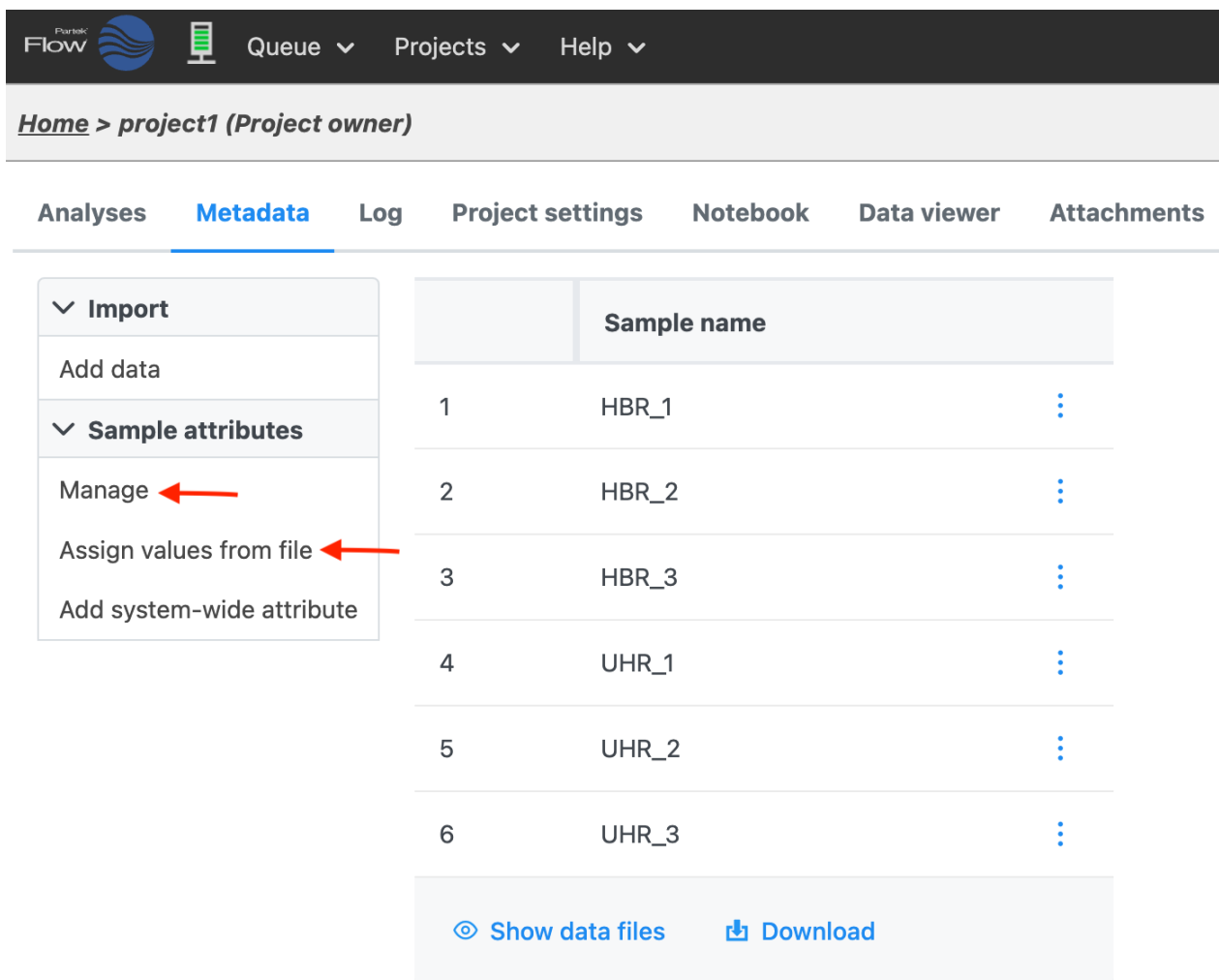
Upon successfully importing data, there will be a circular data node in the project.



Right click on the data node to either delete this node, files, or change data type.



Next, click on the "Metadata" tab to add metadata for the samples. Under the "Sample attributes" sections, users can manually add metadata or assign it from a file. This example will demonstrate manually adding metadata by clicking on "Manage".



Partek Flow Queue Projects Help

[Home](#) > [project1](#) (Project owner)

Analyses **Metadata** Log Project settings Notebook Data viewer Attachments

▼ Import

Add data

▼ Sample attributes

Manage ←

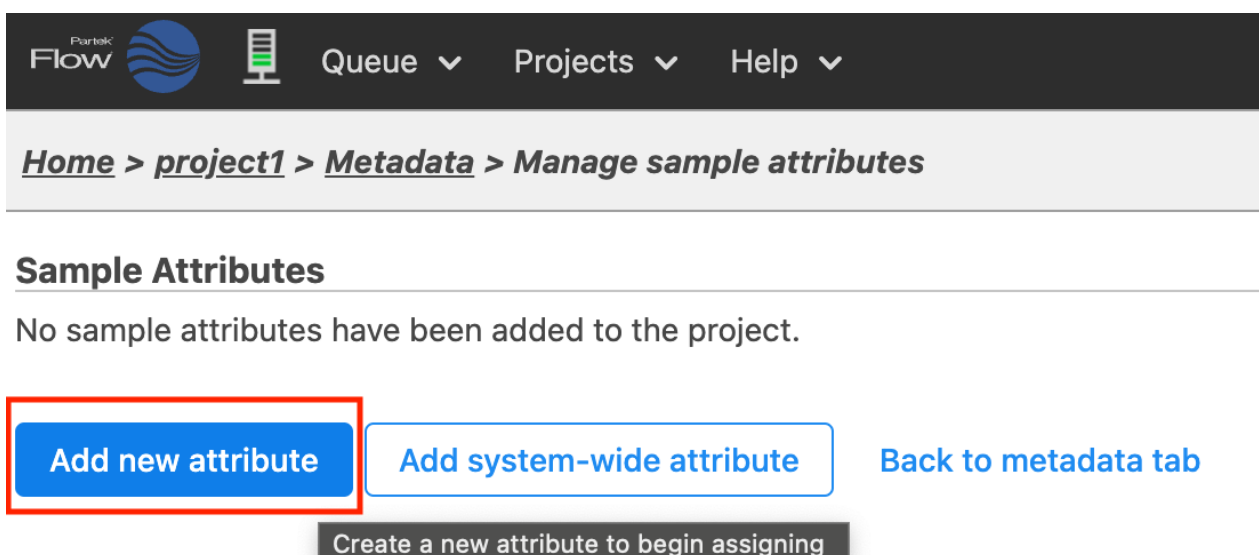
Assign values from file ←

Add system-wide attribute

	Sample name	
1	HBR_1	⋮
2	HBR_2	⋮
3	HBR_3	⋮
4	UHR_1	⋮
5	UHR_2	⋮
6	UHR_3	⋮

👁 Show data files 📄 Download

In the next page, select "Add new attribute".



Partek Flow Queue Projects Help

[Home](#) > [project1](#) > [Metadata](#) > [Manage sample attributes](#)

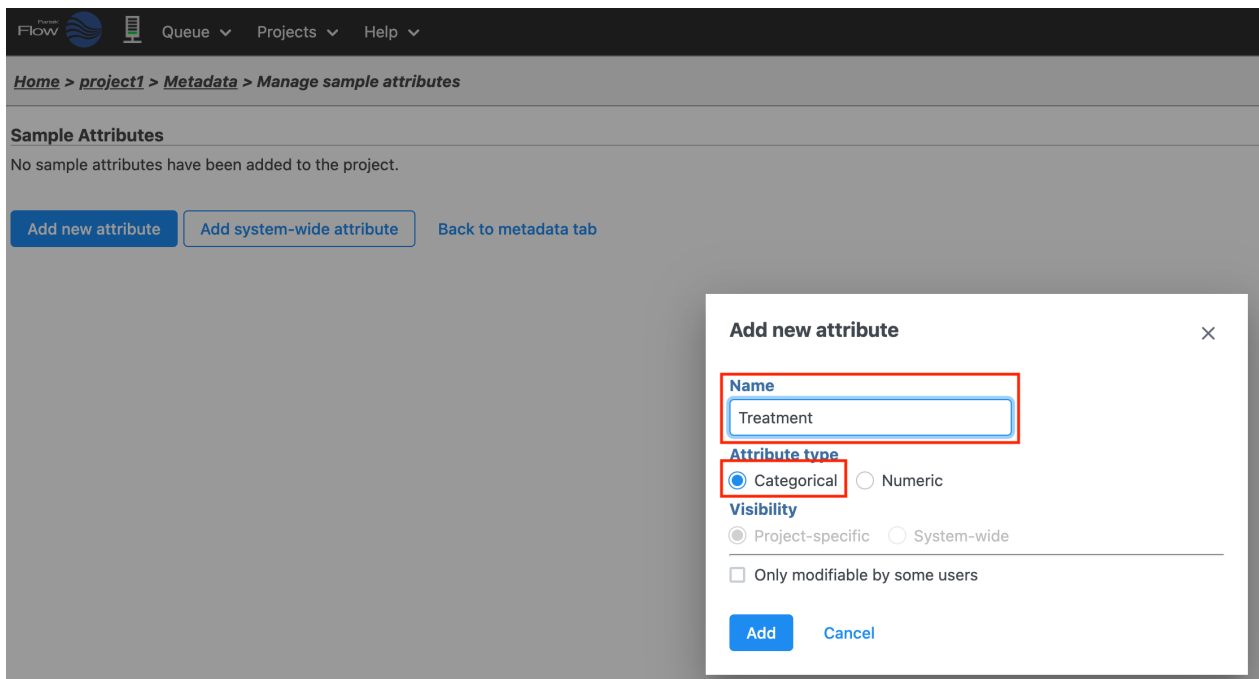
Sample Attributes

No sample attributes have been added to the project.

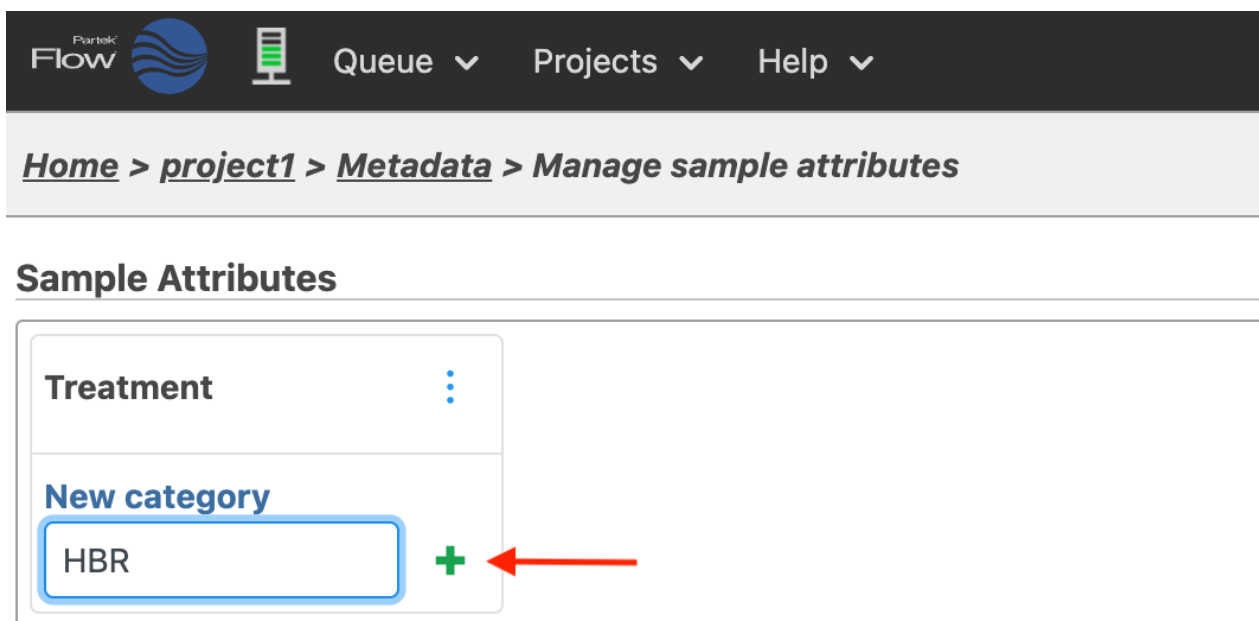
Add new attribute Add system-wide attribute Back to metadata tab

Create a new attribute to begin assigning

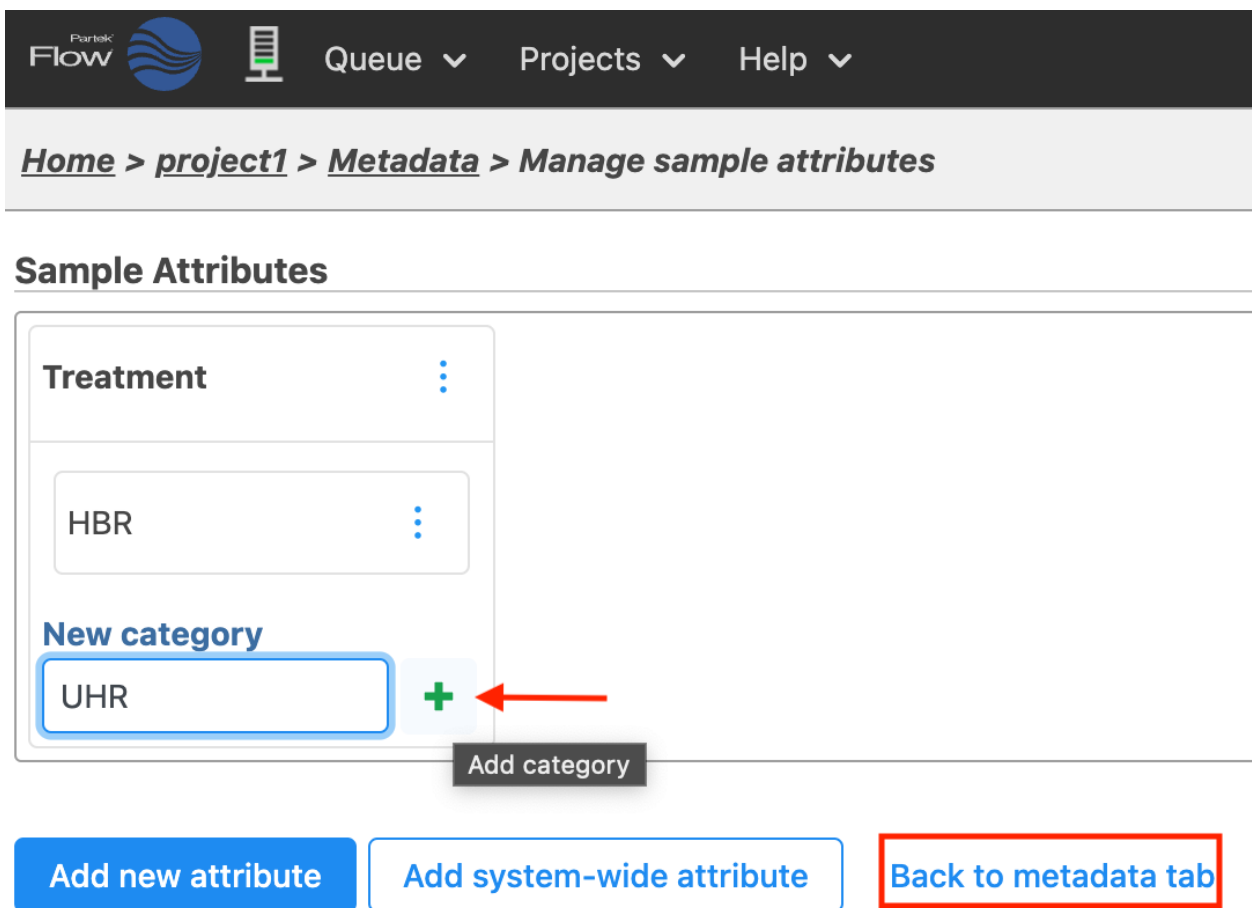
In the dialogue box that appears, name this attribute (think of an attribute as a variable) "Treatment" so that users can distinguish the treatment group in which each sample belong. Be sure that "Categorical" is selected as this attribute type (ie. treatment group is categorical). Click "Add" when ready.



Then, under the "New category" box, enter the first treatment group (ie. HBR). Be sure to click the green "+" to add it.



After that, add the second treatment group (ie. UHR) and click on the green "+" to add. Click the "Back to metadata tab" when finishing adding treatment groups.



Partek Flow

Queue ▾ Projects ▾ Help ▾

Home > project1 > Metadata > Manage sample attributes

Sample Attributes

Treatment

HBR

New category

UHR

+



Add category

Add new attribute

Add system-wide attribute

Back to metadata tab

Hit the "Assign values" tab.

 Queue ▾ Projects ▾ Help ▾

Home > project1 (Project owner)

Analyses Metadata Log Project settings Notebook Data viewer Attachments

▼ Import

Add data

▼ Sample attributes

Manage

Assign values

Assign values from file

Add system-wide attribute

	Sample name	Attributes
		Treatment
1	HBR_1	N/A
2	HBR_2	N/A
3	HBR_3	N/A
4	UHR_1	N/A
5	UHR_2	N/A
6	UHR_3	N/A

Apply changes Discard changes

Then, select the appropriate treatment for each sample using the drop down box. Click on "Apply changes" when finished and then the "Analyses" tab to go back to the analysis.

Partek Flow

Queue ▾ Projects ▾ Help ▾

Home > project1 (Project owner)

Analyses Metadata Log Project settings Notebook Data viewer Attachments

▼ Import

Add data

▼ Sample attributes

Manage

Assign values

Assign values from file

Add system-wide attribute

	Sample name	Attributes
		Treatment
1	HBR_1	N/A
2	HBR_2	N/A HBR UHR
3	HBR_3	N/A
4	UHR_1	N/A
5	UHR_2	N/A
6	UHR_3	N/A

Apply changes Discard changes

Click on a data node to see a menu of tasks that can be performed. For instance, the first step in analyzing high throughput sequencing data from FASTQ files is to perform pre-alignment QC.

Partek Flow

Queue ▾ Projects ▾ Help ▾

Home > project1 (Project owner)

Analyses Metadata Log Project settings Notebook Data viewer Attachments

Venn diagram

Download data (453 MB)

× mRNA

▼ Import

Add data

▼ QA/QC

Pre-alignment QA/QC

ERCC (Bowtie)

ERCC (BWA)

Filter contaminants (Bowtie 2)

> Pre-alignment tools

> Metagenomics

> Aligners

> Quantification

> Filtering

> Assemblers

> 10x Genomics

> Pipelines

Note

In Partek Flow, data nodes are round and task nodes are rectangular. Running tasks are light blue rectangles with a status bar inside. Once the task is complete, the rectangle turns into a darker shade of blue.

