**Get Started**

Summary

Set Environment

Install SSH Client on Your PC Download NetLogo to HPC

Run Experiment

Set Model BehaviorSpace

Revise and Run create\_xmls.sh

Revise and Run submit\_jobarray.slurm

Merge CSV Results Other Notes

**Cheat Sheet**

# **G et Started**

## **Summary**

The main idea is to run NetLogo's [BehaviorSpace](http://ccl.northwestern.edu/netlogo/docs/behaviorspace.html#advanced) in ["headless" mode](http://ccl.northwestern.edu/netlogo/docs/behaviorspace.html#running-from-the-command-line). Experiments in BehaviorSpace are split into a number of separate simulations, each of which is submitted to HPC as a separate job and run in parallel.

Four steps are required to run NetLogo models on HPC:

1. Install an [SSH](https://en.wikipedia.org/wiki/Secure_Shell) client to connect HPC (For Mac OS users, this is not required).
2. Download NetLogo software and unzip it to your project directory on HPC.
3. Add an experiment in the BehaviorSpace of your NetLogo model.
4. Make a copy of the templates in this repository, revise and run your model.

Steps 1 and 2 are to set up work environment and only need to be done once.

## **Set Environment**

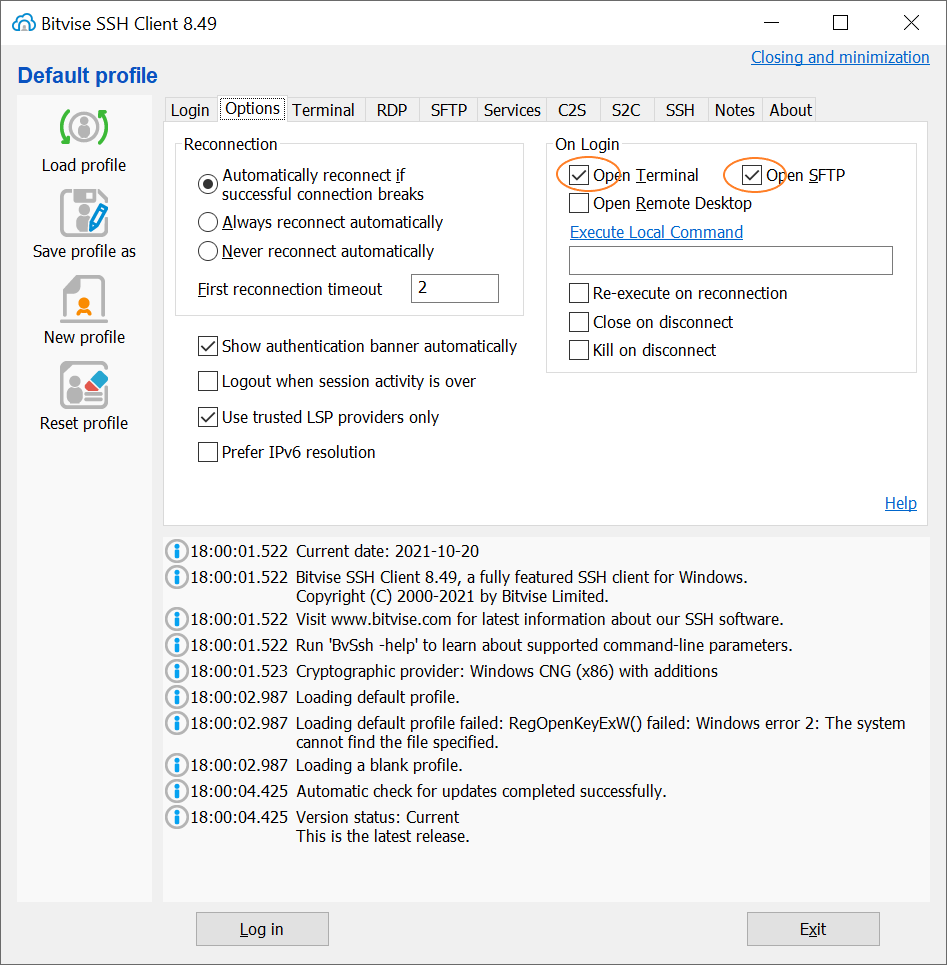
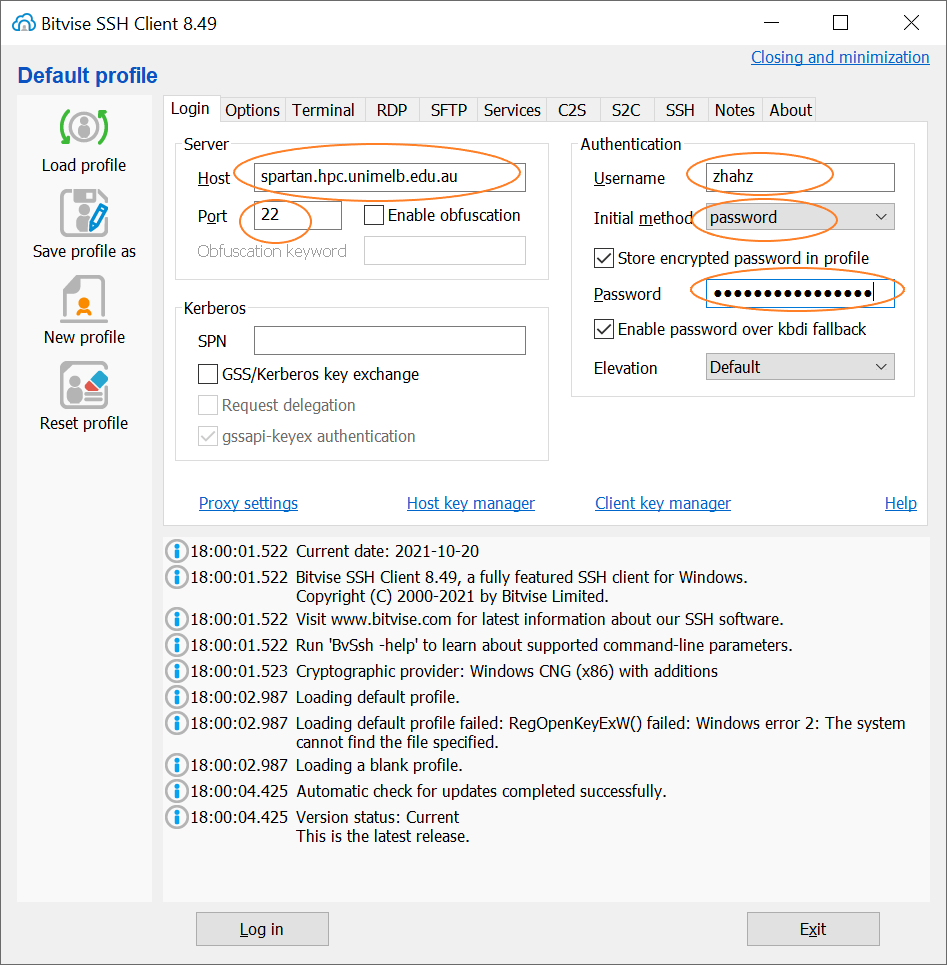
### **Install SSH Client on Your PC**

This part is only required for Windows users. Mac (OS X) already has an SSH client built-in, so Mac users can skip this step.

1. Install an SSH client such as [PuTTY](http://www.putty.org/), [Bitvise](https://www.bitvise.com/ssh-client-download), or [MobaXTerm](http://mobaxterm.mobatek.net/download-home-edition.html). Here we use [Bitvise SSH Client](https://www.bitvise.com/ssh-client-download) as an example.
2. Set up Bitvise SSH client

Tab **[Login]**: Set **Host** as spartan.hpc.unimelb.edu.au (change here to use the host by your institute), **Port** as 22 , **Username** as your username , **Initial method** as password , **Password** as your password.

Tab **[Options]**: Tick **Open Terminal** and **Open SFTP**.



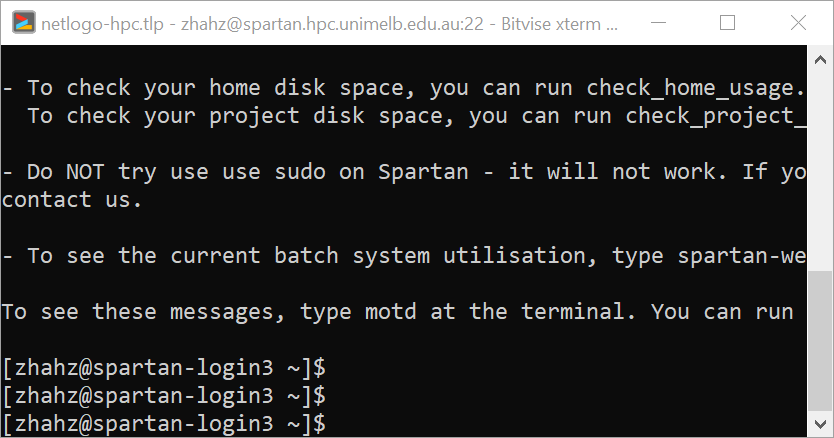
1. Save profile

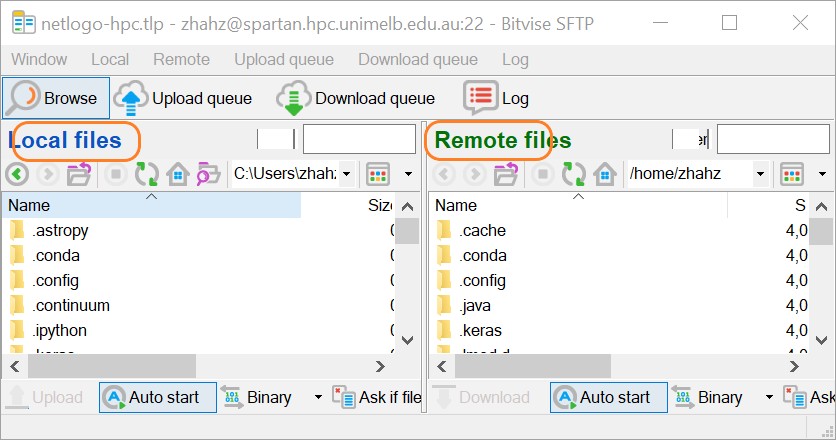
Click [**Save profile**] on the left panel, so that next time you do not need to type all these settings.

1. Log in Spartan

Click [**Log in**] button at the bottom, type your password and click [**OK**] to login. This should open a command prompt window and a SFTP window.

The command prompt is where you type and run your scripts. The SFTP window provides a graphical user interface where you can create/copy/delete files and folders, upload files to your HPC by dragging files from left to right, and download files to your laptop by dragging files from right to left.





### **Download NetLogo to HPC**

In this example, we download NetLogo to this example folder

/data/gpfs/projects/punim1439/workflow/netlogo\_hpc . In th e SFTP window, right click the mouse and Create Folder netlogo\_hpc.

Then, in the command line,

* 1. Run

cd /data/gpfs/projects/punim1439/workflow/netlogo\_hpc

to change current directory to /data/gpfs/projects/punim1439/workflow/netlogo\_hpc .

* 1. Run

wget https://ccl.northwestern.edu/netlogo/6.2.0/NetLogo-6.2.0-64.tgz

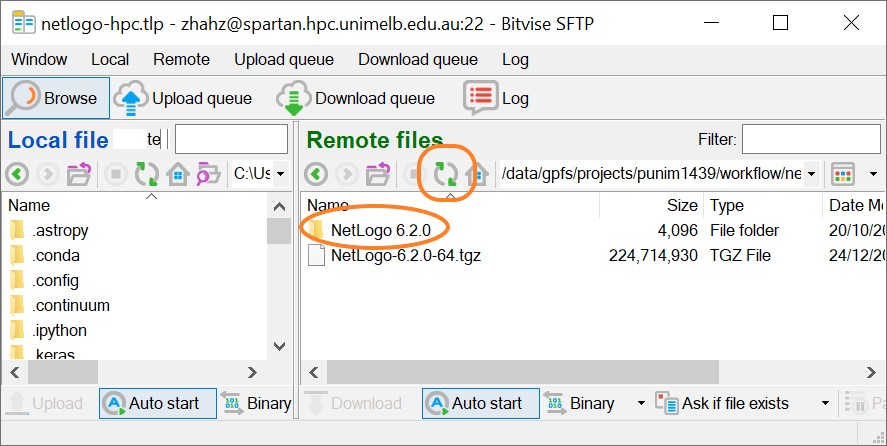
to download NetLogo installation file to current directory.

* 1. Run

tar -xzf NetLogo-6.2.0-64.tgz

to install (unzip) NetLogo to current directory.

Click **Refresh**, and you should be able to see the NetLogo 6.2.0 folder.



💡**Tips**:

Copy and paste in command prompt: **Right Click** mouse🖱 in the command prompt to paste content from the clipboard.

Press up the arrow key⬆ or down arrow key ⬇ on the keyboard to recall your command history.

## **Running Experiments**

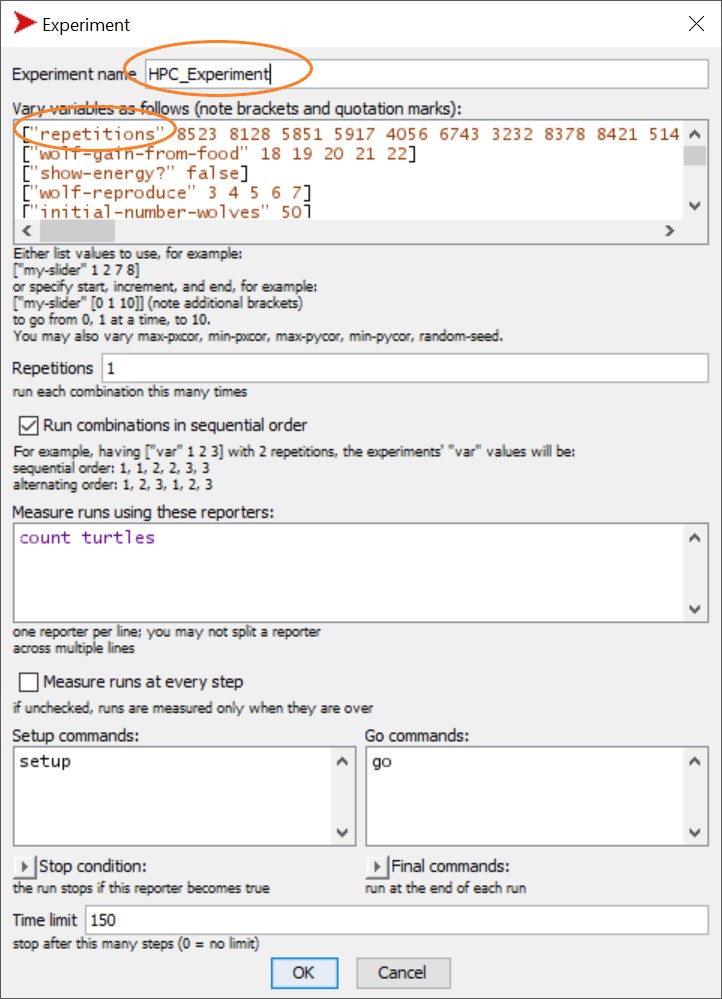
### **Set Model BehaviorSpace**

1. We used a

Wolf\_Sheep\_Predation.nlogo

model as an example.

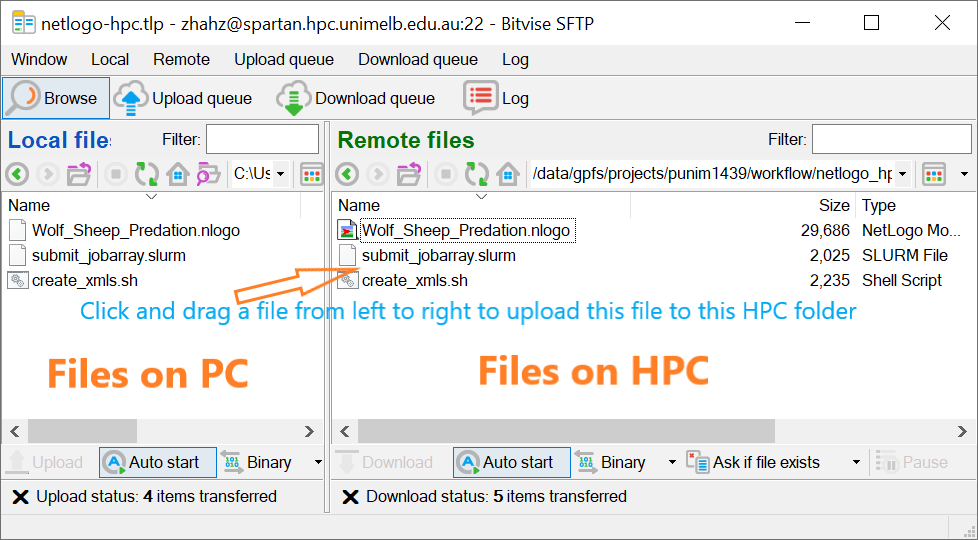
This model is an adjusted version of the NetLogo sample model available in the Netlogo library: NetLogo 6.2.0/app/models/Sample Models/Biology/Wolf Sheep Predation.nlogo. We created an HPC\_Experiment in the BehaviorSpace, added a global variable ‘repetitions’ with 100 values, and removed the line in the Netlogo code that creates the user-message "The sheep have inherited the earth".



1. Upload Wolf\_Sheep\_Predation.nlogo , the HPC folder.

create\_xmls.sh

and to



💡**Tips**:

If your model is on GitHub, clone the repo (for example

https://github.com/JTHooker/COVIDModel ) directly to HPC using:

git clone https://github.com/JTHooker/COVIDModel

### **Revise and Run**

create\_xmls.sh

1. Edit

create\_xmls.sh

using a text editor (notepad++, notepad, etc.)

BEHAVIORSPACE\_NAME= 'HPC\_Experiment'

submit\_jobarray.slurm

NETLOGO\_MODEL= '/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_S

heep\_Predation/Wolf\_Sheep\_Predation.nlogo'

1. End of Line (EOL) Conversion

From the Bitvise command line, change directory to Wolf\_Sheep\_Predation :

cd /data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation

Then, run

sed -i.bak 's/\r$//g' create\_xmls.sh

to convert Windows (CR LF) line ending to Unix (LF)

1. Run

bash create\_xmls.sh

From Bitvise command line, run

bash create\_xmls.sh

to create xmls folder and 100 xml files under this folder.

💡**Tips**:

MS-Windows to Unix like operation systems use different End of Line (EOL), which can create errors.

If you want to view line endings in Notepad++, click menu **View > Show Symbol > Show All Characters**, you will see that Windows has line ending with invisible characters **CRLF**, while Unix has **LF**. Click menu **Edit > EOL Conversion > Unix (LF)** to convert MS-Windows to Unix EOL, as HPCuses Unix-like operation systems.

Command does the same thing, using string editor

sed -i.bak 's/\r$//g' create\_xmls.sh

to convert EOL of create\_xmls.sh to Unix removing all **CR**, and the original file is backed up

as submit\_jobarray.slurm.bak .

submit\_jobarray.slurm

### **Revise and Run**

1. Edit

submit\_jobarray.slurm

(using a text editor notepad++, notepad, etc.).

are script directive for the HPC. This script creates a job array of **100** jobs. Each job requires **1** computer node and **8** CPU cores on the **snowy** cluster for a maximum job wall time of **2** hours. When all jobs are ended, an email notification is sent to –mail-

#SBATCH

#SBATCH

--mail-type

user. In

directive, --qos , -A , --job-name , --mail-user ,

are

optional, and can be deleted.

BASE\_FOLDER: current directory of submit\_jobarray.slurm , and the upper directory of

xmls folder.

NETLOGO\_SH: file path of netlogo-headless.sh under NetLogo 6.2.0 directory.

NETLOGO\_MODEL: file path of Wolf\_Sheep\_Predation.nlogo OUTPUT\_FOLDER: name of output folder.

1. End of Line (EOL) Conversion From Bitvise command line, run

sed -i.bak 's/\r$//g' submit\_jobarray.slurm

1. Run

sbatch submit\_jobarray.slurm

sbatch submit\_jobarray.slurm

to submit 100 jobs to the HPC. The entered email address will receive an email when all jobs are completed.

💡**Tips**:

Run username.

squeue -u yourusername

to see current jobs, replacing

with your

yourusername

Run scancel -n wolf\_sheep\_predation to cancel a job, replacing

wolf\_sheep\_predation with the value after

SBATCH --job-name=

submit\_jobarray.slurm ).

Run spartan-weather to see usage of all partitions (optional). Run clear to clear screen.

Run exit to quite command line.

1. Move all slurm\_\*.out files to slurm folder (optional) When all jobs have finished, run

(file

cd /data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation mkdir -p slurms

mv ./slurm-\*.out ./slurms/

to create a folder slurms, and move all slurm-\*.out files to slurms folder.

### **Merge CSV Results**

cd

/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation/outputs

awk '(NR < 8) || (FNR > 7)' \*\_table\_\*.csv > MergedResults.csv

This will create a file as the final output file.

MergedResults.csv

## **Other Notes**

1.



cd

Change directory command is to avoid always typing the absolute path when running script files.

cd /data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation

bash create\_xmls.sh

sbatch submit\_jobarray.slurm

cd outputs

awk '(NR < 8) || (FNR > 7)' \*\_table\_\*.csv > MergedResults.csv

is the same as using

bash

/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation/crea te\_xmls.sh

sbatch

/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation/subm it\_jobarray.slurm

awk '(NR < 8) || (FNR > 7)'

/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation/outp uts/\*\_table\_\*.csv >

/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation/outp uts/MergedResults.csv

1. In the command prompt, put file path or directory path in example



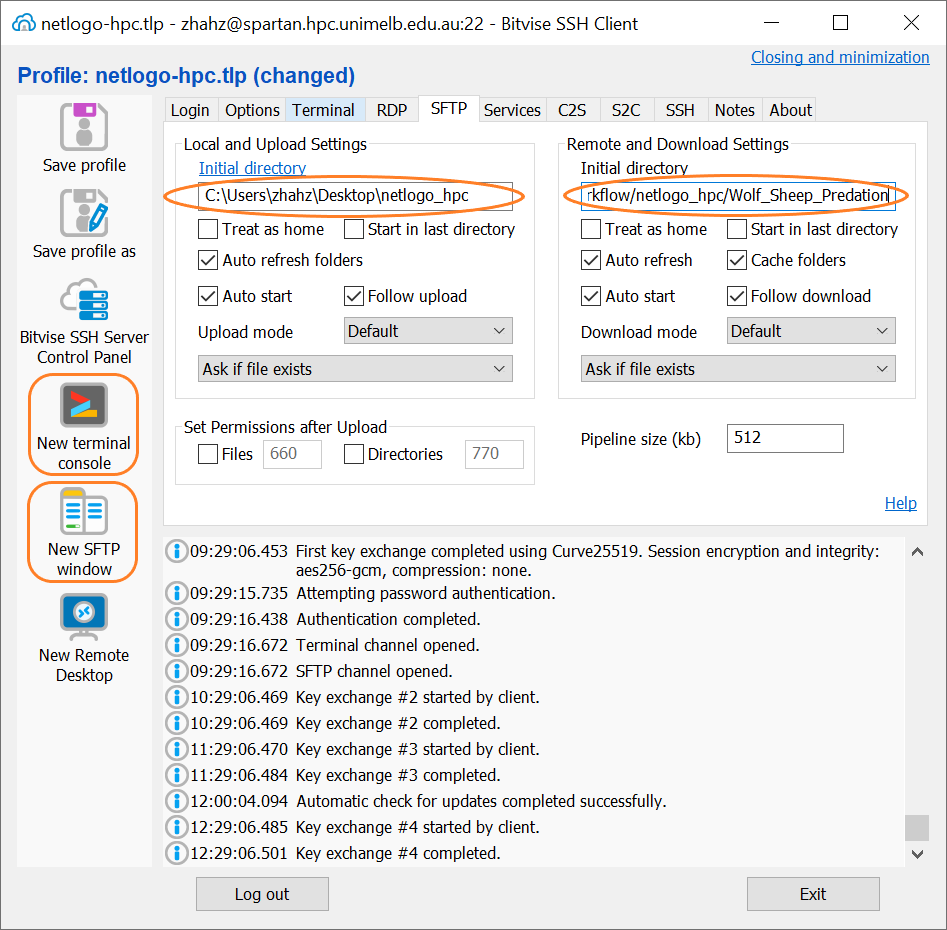
“ ”

if filename includes space. For

cd “/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/NetLogo 6.2.0”

1. Bitvise

Click **[New terminal console]** to open a new command window. Click **[New SFTP window]** to open a new SFTP window. Set the **Initial directory** in Tab **[SFTP]** and Save profile, to specify initial directories for your new SFTP windows.



1. NetLogo RAM

To run models that require large memory, you need to change NetLogo's RAM of Java virtual machine (JVM).

Make a copy of netlogo-headless.sh (e.g. netlogo-headless-10g.sh)

cd "/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/NetLogo 6.2.0" cp netlogo-headless.sh netlogo-headless-10g.sh

Edit netlogo-headless-10g.sh : Line 15, Change **-Xmx10240m** to **-Xmx10g** to increase 1GB RAM to 10GB RAM.

JVM\_OPTS=(-Xmx10g -XX:+UseParallelGC -Dfile.encoding=UTF-8)

Notes: You can either edit

netlogo-headless-10g.sh

line on command prompt by running

using any text editors, or edit in

nano netlogo-headless-10g.sh

After editing, press <Ctrl+X> to exit, type <Y> to save changes, then press <Enter> to overwrite the file.

1. NetLogo extensions

If your model requires an extension which is not a default extension of NetLogo software, the extension should be copied to the same folder of the NetLogo model or can be placed in the extensions folder in the NetLogo extensions directory. Refer [here](https://ccl.northwestern.edu/netlogo/docs/extensions.html) for where to find extensions.

For example, we can copy rngs folder from

C:\Program Files\NetLogo

on our laptop to

6.2.0\app\extensions\.bundled\rngs

/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/NetLogo 6.2.0/app/extensions/.bundled/rngs on HPC.

1. Single run

If your experiment only has **one run** that cannot be split (Note the of

HPC\_Experiment

has 100 runs), or you just want to run your model by submitting one job to HPC, then you can simply save the following script as

Wolf\_Sheep\_Predation.nlogo

(ℹuse Unix EOL), and run

submit\_single\_job.slurm

sbatch submit\_single\_job.slurm

after you Set Model BehaviorSpace, you do not need to run Revise and Run

Revise and Run submit\_jobarray.slurm

create\_xmls.sh ,

and Merg

CSV Results.

# -- file submit\_single\_job.slurm --

#!/bin/bash

#SBATCH --nodes=1

#SBATCH --partition interactive

#SBATCH --time 1:00:00

#SBATCH --cpus-per-task=8

module load java

cd "/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation" "/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/NetLogo 6.2.0/netlogo- headless.sh" \

--model "Wolf\_Sheep\_Predation.nlogo" \

--experiment "HPC\_Experiment" \

--table "output\_file.csv"

You can also run NetLogo headless mode on Windows PC (if JAVA\_HOME has been set or system PATH has included java.exe), using

cd "C:\Users\zhahz\Desktop\netlogo\_hpc"

"C:\Program Files\NetLogo 6.2.0\netlogo-headless.bat" ^

--model "Wolf\_Sheep\_Predation.nlogo" ^

--experiment "HPC\_Experiment" ^

--table "output\_file.csv"

1. 💡 Use [create\_xmls\_nested.sh](https://github.com/melbhz/netlogo-hpc/blob/main/workflow/create_xmls_nested.sh) to split model by more than one variable
   * BEHAVIORSPACE\_NAME='HPC\_Experiment'
   * NETLOGO\_MODEL='/data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation/Wolf Sheep Predation HPC.nlogo'
   * **SPLIT\_BY\_VARIABLES**=("wolf-gain-from-food" "wolf-reproduce") to split the experiment by two variables "wolf-gain-from-food" and "wolf-reproduce"

# **Cheat Sheet**

# change work directory

cd /data/gpfs/projects/punim1439/workflow/netlogo\_hpc/Wolf\_Sheep\_Predation

# create experiments

sed -i.bak 's/\r$//g' create\_xmls.sh bash create\_xmls.sh

# check which partition has more available CPUs spartan-weather

# submit jobs

sed -i.bak 's/\r$//g' submit\_jobarray.slurm sbatch submit\_jobarray.slurm

# check job status squeue -u yourusername

# clean log files mkdir slurms

mv ./slurm-\*.out ./slurms/

# merge results cd outputs

awk '(NR < 8) || (FNR > 7)' \*\_table\_\*.csv > MergedResults.csv

# cancel job

scancel -n wolf\_sheep\_predation