Get Started

Summary

The main idea is to run NetLogo's BehaviorSpace in "headless" mode. 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 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, Bitvise, or MobaXTerm.

   Here we use Bitvise SSH Client 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**.
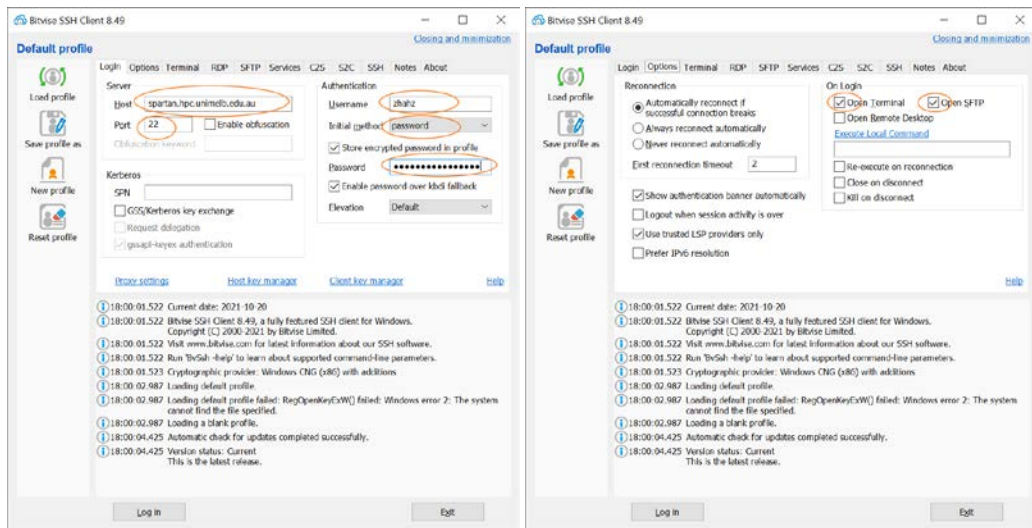
3. Save profile

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

4. 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.
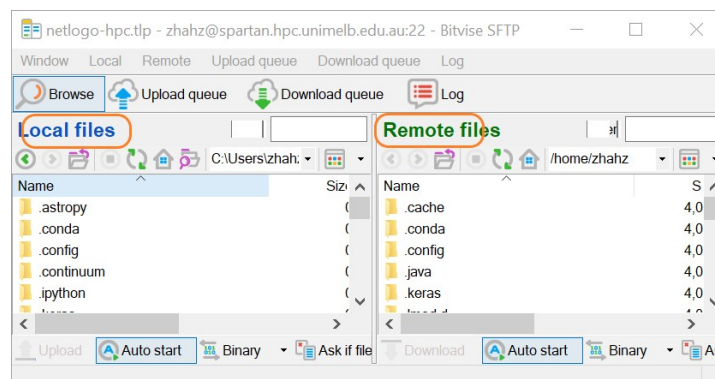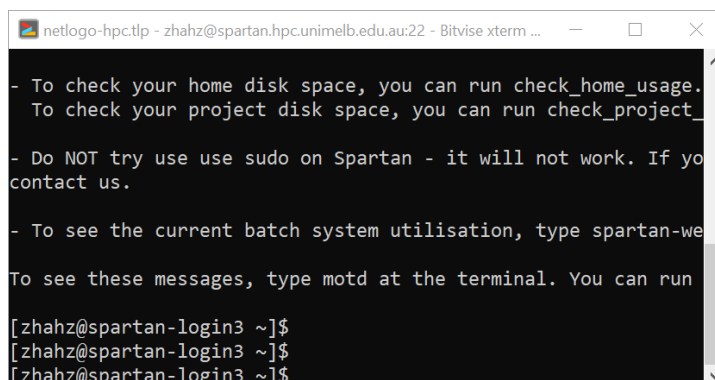
Download NetLogo to HPC

In this example, we download NetLogo to this example folder `/data/gpfs/projects/punim1439/workflow/netlogo_hpc`. In the 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`.

2. Run

   ```
   wget  https://ccl.northwestern.edu/netlogo/6.2.0/NetLogo-6.2.0-64.tgz
   ```
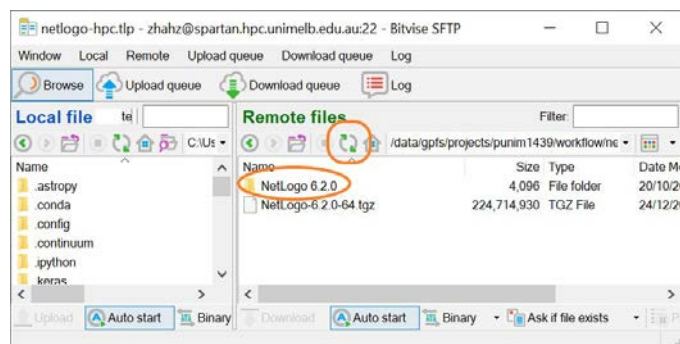
   to download NetLogo installation file to current directory.

3. 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".

2. Upload `Wolf_Sheep_Predation.nlogo`, `create_xmls.sh` and `submit_jobarray.slurm` to the HPC folder.
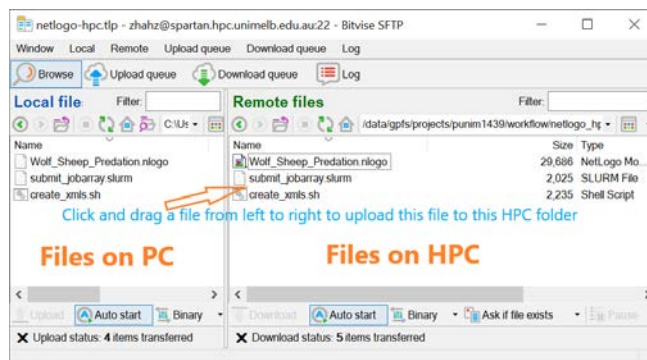
💡**Tips**:

If your model is on GitHub, clone the repo (for example `https://github.com/JTHooker/COVIDModel`) directly to HPC using:

```
git clonehttps://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'`
   - NETLOGO_MODEL= `'/data/gpfs/projects/punim1439/workflow/netlogo_hpc/Wolf_Sheep_Predation/Wolf_Sheep_Predation.nlogo'`
2. 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)

3. 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 `sed -i.bak 's/\r$//g' create_xmls.sh` does the same thing, using string editor to convert EOL of `create xmls.sh` to Unix removing all **CR**, and the original file is backed up as `submit_jobarray.slurm.bak`.

Revise and Run `submit_jobarray.slurm`

1. Edit `submit jobarray.slurm` (using a text editor notepad++, notepad, etc.).

   ◇ `#SBATCH` 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-user. In `#SBATCH` directive, `--qos`, `-A`, `--job-name`, `--mail-user`, `--mail-type` 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.

2. End of Line (EOL) Conversion

   From Bitvise command line, run

```
sed -i.bak 's/\r$//g' submit_jobarray.slurm
```

3. 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.

- Run `squeue -u yourusername` to see current jobs, replacing `yourusername` with your username.
- Run `scancel -n wolf_sheep_predation` to cancel a job, replacing `wolf_sheep_predation` with the value after `SBATCH --job-name=` (file `submit_jobarray.slurm`).
- Run `spartan-weather` to see usage of all partitions (optional).
- Run `clear` to clear screen.
- Run `exit` to quite command line.

4. Move all slurm_*.out files to slurm folder (optional)

When all jobs have finished, run

```
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 `MergedResults.csv` as the final output file.

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
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
```

2. In the command prompt, put file path or directory " " if filename includes space. For path in example

```
cd "/data/gpfs/projects/punim1439/workflow/netlogo_hpc/NetLogo 6.2.0"
```

3. 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.
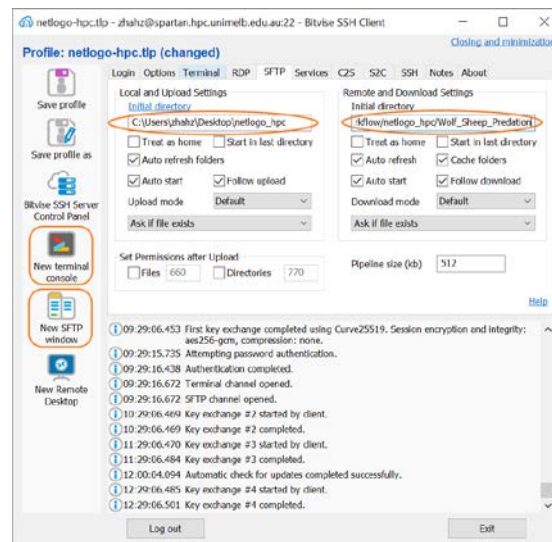
4. NetLogo RAM

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` using any text editors, or edit in line on command prompt by running

```
nano netlogo-headless-10g.sh
```

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

5. 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](#) for where to find extensions.

   For example, we can copy `rngs` folder from `C:\Program Files\NetLogo 6.2.0\app\extensions\.bundled\rngs` on our laptop to `/data/gpfs/projects/punim1439/workflow/netlogo_hpc/NetLogo 6.2.0/app/extensions/.bundled/rngs` on HPC.

6. Single run

   If your experiment only has **one run** that cannot be split (Note the `HPC Experiment` of `Wolf_Sheep_Predation.nlogo` 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 `submit_single_job.slurm` (🛈 use Unix EOL), and run

   ```
   sbatch submit_single_job.slurm
   ```

   after you [Set Model BehaviorSpace,](#) you do not need to run [Revise and Run](#) [create_xmls.sh](#) , [Revise and Run](#) [submit_jobarray.slurm](#) 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"
```

7. 💡 Use create_xmls_nested.sh to split model by more than one variable
   o BEHAVIORSPACE_NAME='HPC_Experiment'
   o NETLOGO_MODEL='/data/gpfs/projects/punim1439/workflow/netlogo_hpc/Wolf_Sheep_Predatio
     n/Wolf Sheep Predation HPC.nlogo'
   o **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
```