

Using the Cirrus computing facility

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2024-03-26

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1 Preliminaries

You will need to [create an account](#) on the [SAFE website](#) and ask [Brendon](#) to add you to project **d422 (Nanomaterials)**. Once added, this project will be listed under the Projects tab of the

website and a user account created for you on Cirrus. An initial password for this account will be emailed to you. Your username is listed as `user@cirrus` under the `Login` `accounts` tab.

Further information (registration tips) During registration, you will be asked to select an institution from a bizarrely sorted¹ list (University of St Andrews is near the bottom) and optionally provide a default `ssh` public key used for new login accounts such as the one created for Cirrus, although this can easily be done after account creation (see below). I recommend staying subscribed to user emails which include important service changes and notifications; you can filter these optional mailings from `Your details` → `Update email settings`. Since late 2023 it is also recommend to setup MFA for you account with an authenticator app (`Your details` → `Set 2 factor token`).

N.B. all login details for the `SAFE` website, including any MFA, are entirely *separate* from those used to access the Cirrus facility itself.

2 Accessing Cirrus

2.1 Authentication: Adding SSH credentials and MFA token

To access Cirrus, you need two credentials: an SSH key pair (protected by a passphrase) and a time-based on-time passcode ('TOTP code' or 'MFA token').

To configure `ssh`-keys and MFA token, navigate to `Login` `accounts` on the `SAFE` and select your user. If you did not add a default `ssh` key when creating an account, or wish to add another, e.g., for a second device, you can do so by clicking the red `Add Credential` button, `Credential Type`: `ssh public key` and upload the file containing your public key or paste its contents directly into the input box before pressing `Add`. For the MFA token, click `Set MFA-Token`. A QR code will be displayed which you can scan with you phone's camera from within an authenticator app such as Google or Microsoft Authenticator. Enter the code generated and press `set` to confirm the Token.

Further information (generating SSH keys) For those who have not used `ssh` before, the `OpenSSH ssh-keygen` tool is the standard way to create `ssh` private/public key pairs on Mac, Linux and Windows. Note the location to which the public key (`.pub`) is installed. The tool will prompt you for a password when creating the key (this is entirely separate from the `SAFE` website and `cirrus` login passwords)—enter nothing to skip this addition layer of password protection.

2.2 First-time login

In all of the following `user` refers to your username displayed as `user@cirrus` in the `Login` `accounts` tab of the `SAFE` website.

Having adding your public key to your login account you can connect to Cirrus using

```
$ ssh user@login.cirrus.ac.uk
```

You will be prompted to enter a TOTP code generated by the app you set up above. That's it! The commands `logout`, `exit` or `Ctrl+D` may be used to close the connection to Cirrus at any time. There appears to be a short window after closing the connection during which a new connection from the same device will not require a new TOTP code, i.e., the SSH credentials suffice.

¹The arrangement is something like: English universities sorted alphabetically by placename (i.e. ignoring 'University', 'The', 'of'), then Scottish, then Welsh, then Irish and finally other UK and non-UK research and commercial institutions.

Further information (SSH configuration) If you installed your private–public ssh key in a non–standard location, or have multiple keys installed on your system, it may be necessary to specify the path to the relevant private key using the `-i` option of ssh e.g. `$ ssh -i ~/my_keys/cirrus_rsa user@login.cirrus.ac.uk`. To streamline future connections you can add an entry to your local ssh configuration file (`~/.ssh/config`) such as

```
1 Host cirrus
2     HostName login.cirrus.ac.uk
3     User user
4     IdentityFile ~/my_keys/cirrus_rsa
```

The command `ssh cirrus` (or `scp...cirrus:...`) can then be used to login (or copy) to Cirrus as user. A second useful snippet is

```
1 Host *
2 ControlMaster auto
3 ControlPath ~/.ssh/sockets/%h-%p-%r
```

This allows ssh connections to be reused, in particular saving time and the need to enter a password when using scp if you already have an ssh session to Cirrus running.

3 Working with files on Cirrus

3.1 Filesystem structure

As of March 2024, there are two relevant locations on Cirrus you have write access to as user:

- A home directory, `/home/d422/d422/user`, for personal files and configuration. The compute nodes do not have access to this directory, so you won't be using this much.
- A work directory, `/work/d422/d422/user`. When a job is run on cirrus, this directory is added to a mount point accessible by the compute nodes. It is hence the relevant location for any software installation as well as scripts, input and output data.

Note that Cirrus does *not* backup any data. In addition, with large system upgrades or filesystem restructuring in the past the contents of the user home and work directory has been archived (for example, there is currently a read-only directory `home-archive/d422/` containing data before March 2022). You may wish to create a symlink as `$ ln -s /work/d422/d422/user work` in your user directory if one does not already exist.

3.2 Transferring files

In addition to interactive access to cirrus the `scp` command (or equivalent file transfer utility e.g. `rsync`) can be used to transfer data to and from Cirrus. For example, the command

```
$ scp -r test_scripts user@login.cirrus.ac.uk:remote_test_scripts
```

copies a local directory `test_scripts` to a directory called `remote_test_scripts` in your user's *home* (not *work*) directory on Cirrus, and

```
$ scp -r user@login.cirrus.ac.uk:remote_test_scripts test_scripts
```

does the reverse. Note both of the above commands should be run in a local session; you can't scp from a Cirrus login node to your own machine unless you have a ssh server running on your machine.

3.3 Using git

git is provided on cirrus and it is likely you will want to clone a repository with relevant code or data (scp is more appropriate for large files). For example, to clone the OQuPy repository using HTTPS,

```
$ git clone https://github.com/tempoCollaboration/OQuPy.git
```

or, using SSH,

```
$ git clone git@github.com:tempoCollaboration/OQuPy.git
```

Using SSH has the convenience of passwordless access to private repositories, but requires an SSH key-pair on your Cirrus home (or work) directory (use `ssh-keygen` as above) with the public added to your Github account or relevant host.

4 Using python on Cirrus

4.1 Overview

Early May 2023 there was a significant upgrade to the Python installations on Cirrus.² There are now a number of versioned Miniconda/Anaconda modules available on the login and compute nodes providing the common suite of scientific packages—`numpy`, `scipy`, `matplotlib` etc.—plus the ability to install additional packages from PyPI or the conda repositories. For those who want complete control over their python environments i.e. installed packages and their versions, or to install packages not on PyPI or Conda repositories, a local installation of Miniconda is still recommended, see Section 4.3. Otherwise, the centrally-installed python should be sufficient and Section 4.2 is for you.

4.2 Using the Cirrus python modules (easy)

In addition to the base python-2 and -3 executables,³ Cirrus provides several different python installations or 'modules' with pre-installed packages that you will likely need to run your code.

In order to use a python module it firstly needs to be *loaded*. To list available modules, enter `module avail python`. At the time of writing, this produces

```
$ module avail python
----- /mnt/lustre/indy2lfs/sw/modulefiles -----
python/3.7.16 python/3.8.16-gpu python/3.9.13 python/3.9.13-gpu ...
```

You will typically want to use the latest non-gpu specific installation, in this case `python/3.9.13`. To load the module, run `module load python/X.X.XX`:

²Previously, python was provided by a single Anaconda distribution and the advice was to use a local Miniconda installation (Section 4.3) if additional packages were required. Alongside improving ease of use and reliability I expect performance was a target of the upgrade: the multiprocessing package `mpi4py` and machine learning frameworks `pytorch`, `tensorflow` may benefit from being built specifically for Cirrus hardware (GPUs). This is unlikely to matter to you (but if it sounds like it might, see [Using Python](#)).

³These are available immediately from when you login as `python2` and `python3`, but are without additional packages.

```
$ module load python/3.9.13
```

After loading, the command `python` is aliased to a specific python version and you will have access to all packages provided by the module, e.g.

```
$ python
Python 3.9.12 (main, Apr 5 2022, 06:56:58) # Looks slightly out-dated!
>>> import numpy as np # no ImportError
>>> exit
```

To list all the packages provided by a module, run `pip list` *after* loading it. If this includes all the packages you need, then you are done—you simply need to add `module load python/X.X.XX` in your submission script before any python code is run (Section 5). If not, you will need to create a virtual environment.

4.2.1 Virtual environments

To create a virtual environment based on a Cirrus python module, firstly load the module e.g. `module load python/3.9.13` and then use

```
$ python -m venv --system-site-packages /work/d442/d422/user/my-env
```

Here `user` should of course be replaced by your own login and `my-env` a sensible name for your environment in your work directory (if you plan on having multiple environments you may wish to create a subdirectory). Next, run `extend-venv-activate` on the new environment:

```
$ extend-venv-activate /work/d422/d422/user/my-env
```

This ensures the selected Cirrus python module is loaded and unloaded whenever the environment is activated or deactivated. To use the environment in the current session, activate it using `source`:

```
$ source /work/d422/d422/user/my-env
```

You should notice `(my-env)` appears at the prompt. You can now install additional packages i.e. those not provided by the base set using `pip install` as follows:

```
$ pip install PACKAGE_NAME
```

Once you have finished installing packages, you can leave the virtual environment with `deactivate`. All that needs to be done now is to place the above `source .../my-env` command in your submission script before any python invocation (`module load` is *not* required), see Section 5.

4.3 Local Miniconda installation for python (advanced)

While the central python modules provide a wide array of python packages suitable for many projects, if you need complete control over your development environment it is best to start from an empty python environment. A local Miniconda installation, detailed below, is a reliable way to do this.⁴

⁴This *can* be done using the system-wide python (run `python3 -m venv` without loading a module), but I wouldn't recommend it—changes to the system python will likely break everything.

4.3.1 Installation

Firstly, after logging in to Cirrus navigate to `/work/d422/d422/user` and download Miniconda3 using `wget`:

```
$ wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
```

Run the installer with

```
$ bash Miniconda3-latest-Linux-x86_64.sh
```

Accept the license terms and enter `/work/d422/d422/user/miniconda3` as the install location. At the end be asked if you wish the installer to ‘initialize Miniconda3.’ This appends lines to your `~/.bashrc` to the effect of adding `miniconda3/bin/` to your path and loading the base (default) environment on login. I have seen this fail to work properly in the past, so would suggest answering no unless you are particularly keen to have this ‘convenience’: there is little reason to use python as a user on Cirrus other than to manage environments.

Miniconda environments will need to be loaded by the compute nodes when running jobs. To provide for this, create a script in your work directory called `miniconda-init.sh` (for example) containing the single line:

```
eval "$(/work/d422/d422/user/miniconda3/bin/conda shell.bash hook)"
```

where `user` must of course be replaced by your actual username. This script will be sourced at the start of any job we run on Cirrus and must be given executable permissions:

```
$ chmod +x miniconda-init.sh
```

4.3.2 Environment setup

To create and initialise a python environment called `oqupy` (# indicates a comment):

```
# load base environment (does nothing if already loaded)
$ source miniconda3/bin/activate
# create a new environment using conda
$ conda create --name oqupy
# load the new environment to begin using it ('conda deactivate' to unload)
$ conda activate oqupy
```

Once activated, you can install packages into that environment. The simplest⁵ way to do this is to install the `pip` package manager using `conda install pip` after which packages can be installed using `pip install numpy` (for example) or from a list in a file with `pip install -r requirements.txt`.

5 Running jobs on Cirrus

5.1 Overview

The simplest workflow for running jobs on Cirrus requires two files:

⁵conda can also be used to install packages, but it does not have access to the complete Python Package Index (PyPI) and has less simple syntax for e.g. installing packages from a file. If using both, it is recommended to install conda packages first before installing any packages that conda cannot provide with `pip`.

-
1. A python script (`run-me.py`) containing the code you wish to run. This must be executable (`chmod +x run-me.py`) and contain the python shebang `#!/usr/bin/env python` on the first line.
 2. A submission script (`submit-me.slurm`) containing job options and a command to run the python script. This does not need to be executable, but should contain commands to change to an appropriate working directory and load any required python modules or environments.

Examples for `submit-me.slurm` and `run-me.py` are attached to the end of this document. Both *must* be placed in your user's work directory (or a subdirectory thereof) in order to be accessible by the compute nodes. You should be able to modify these examples for your own purpose. Note `run-me.slurm` is a Shell script in which you can use for loops, redirects and generally any Bash shenanigans to e.g. start `run-me.py` multiple times with different arguments.

Once these scripts are in place, you can submit the job to the Cirrus scheduler using `sbatch`:

```
$ sbatch submit-me.slurm
Submitted batch job ID
```

Here ID is a 7 digit identifier assigned to the job. The job will be placed in a system-wide queue and run when sufficient resource becomes available (if not immediately). `squeue -u user` can be used to view your submitted jobs with the status indicated in the ST column by 'PG' for queued, 'R' for running and 'CG' for cancelling. The last one may be brought about by the command `scancel ID` which tells the schedule to cancel a job you submitted with identifier ID.

Once a job begins to run, any output that you would normally see in your terminal (i.e. `stdout`) is appended to a new file `slurm-ID.out` in the directory you issued the `sbatch` command from. This is useful to monitor the progress of jobs and debug errors. Of course, your python script may also read and write to other files whilst running.

The most common issue running jobs on Cirrus is getting paths linking the submission script, python script and any input/output data correct. Don't worry if things proceed a little by trial and error—in the first two cases at least (i.e. getting the python code running) an incorrect path will cause the job to fail immediately and no resource will be wasted. Personally, I place all my submission scripts in one directory (e.g. `/work/d422/d422/user/submission`), whilst the python script will likely be in a git repository within my work directory (e.g. `.../OQuPy/examples/...`) and I make sure the submission script `cds` to that repository before any python is run.

A summary of the job workflow is given in Fig. 1. Finally, you may wish to edit options for your job in `submit-me.slurm`. The main ones are discussed in Section 5.2 below. The remainder of this section covers some useful tips and information. See also Section 6 which lists some common errors you may encounter and how to fix them.

Further information (login nodes) Note the login nodes themselves have slow I/O and are not suitable for running anything more than basic python scripts and tests!

5.2 Job options

The one option you will almost certainly want to set is the `job-name` (best to call it something sensible as this will be visible in the system-wide queue :). Beyond that, there are two main options you might consider changing:

1. `time` set the maximum length of time (HH:MM:SS) the job can run before being killed. 96 hours is the highest possible value for standard jobs you will have access to.

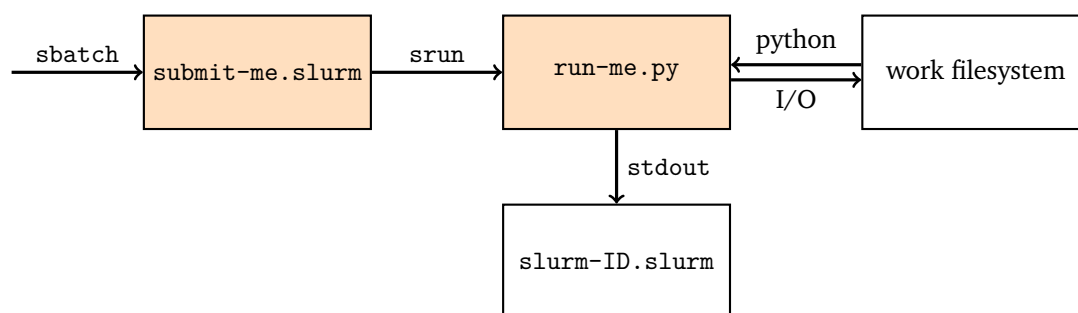


Figure 1: Job workflow

2. `cpus-per-task` is the number of cores assigned to the job—in most cases you'll want to set this to 1; see Section 5.5 for further discussion.

5.3 Passing arguments to your python scripts

Arguments can be passed to your python script from within the submission script as usual, e.g.

```
for T in 0 100 200
do
    echo "Running script at Temperature" $T "K"
    srun --cpu-bind=cores run-simulation.py $T
    sleep 1
done
```

You can also pass arguments to the submission script, referenced using Bash variables "\$1", "\$2",...or the convenient catch-all "\$@". For example, `sbatch submit-me.slurm -mass 70 -freq 123` in conjunction with

```
srun --cpu-bind=cores run-me.py "$@"
```

inside the submission script would result in `"-mass 70 -freq 123"` being passed directly to `run-me.py` (in which these arguments could be accessed via `sys.argv`).

5.4 Resource on Cirrus

Resource usage of a job is measured in Core hours (Corehrs). That's number of cores assigned \times runtime in hours. The **d422** project is allocated a set number of Corehrs per renewal period; you can ask Brendon for the details but this is of the order of 10^5 Corehrs so, as rough guidelines,

- jobs totalling 10s of Corehrs or fewer—run liberally
- jobs totalling 100s of Corehrs or fewer—think carefully before running, at your discretion
- jobs totalling 1000s of Corehrs or more—be very sure before running these, consult Brendon and/or Jonathan

5.5 cpus-per-task

Since vanilla python (i.e. the standard library) does not multithread by default, there is little or no advantage to running scripts on multiple cores and you will typically want to set `cpus-per-task=1` to avoid using unnecessary Corehrs. There are two main exceptions to this:

1. You explicitly code for parallelism in python using the `multiprocessing` module, in which case `cpus-per-task` can be set as high as desired, but note that jobs with low cpu counts are naturally allocated to compute nodes more quickly; during busy hours you will likely find yourself waiting a long time for a job with high CPU counts (e.g. >8).
2. You need to allocate more than ~ 7 GB of memory to your job (see below)

Instead of parallelism within one script then the power of having access to the many processor cores provided by Cirrus is the ability to run many instances of a script at the same time e.g. a simulation with different parameters. This can be done manually by issuing multiple calls to `sbatch` or using another Bash script to execute this command in a `for`-loop.

Further information (job memory) On Cirrus memory aka RAM is allocated according to the number of CPUs used for a task, with approximately 7 GB of memory per CPU. If you need more memory, then you can increase the count `cpus-per-task` in your submission script, but be aware that this also increases the rate at which your job uses Corehrs (e.g. a two hour job with `cpus-per-task=8` costs 16 Corehrs). Hence it is preferable to design your code such that large amounts of memory are not required e.g. by writing intermediary calculations to disk.

A script which can be used to monitor memory usage of a job is attached to this document.

Further information (numpy multithreading) A caveat of the above is that **numpy can leverage multiple threads** for more performant linear algebra using the OpenBLAS or MKL backends (whether this is worth the addition Corehrs: I doubt it). The number of threads can be controlled by setting the `OMP_NUM_THREADS` variable (e.g. `export OMP_NUM_THREADS=1` before a python script is run prevents numpy multi-threading entirely), but I recommend *you do not set this variable* as Cirrus appears to set it appropriately.⁶ The exception I would guess (expert advice needed) is when using `multiprocessing`—there you want to restrict multithreading so each process is not assigned more threads than the corresponding CPU can support.⁷ Note that **other environmental variables** may be relevant.

6 Troubleshooting

⁶Using `threadpoolctl` one can inspect `python -m threadpoolctl -i numpy` on the compute nodes (i.e. via a job).

⁷Since each Cirrus CPU supports two threads with hyperthreading enabled by default, my guess would be that `OMP_NUM_THREADS=2` is ideal.

Common error	Common solutions
<code>/var/.../slurm_script:...cd: ...No such file or directory</code>	The path used by the <code>cd</code> command in your submission script is wrong
<code>slurmstepd:...run-me.py: No such file or directory or slurmstepd:...: Not a directory</code>	The path in your submission script to your python script is wrong (remember to account for any preceding <code>cd</code>)
<code>FileNotFoundError: [Errno 2] No such file or directory:...</code>	A path in your python script is wrong
<code>/usr/bin/env: 'python': No such file or directory</code>	You didn't load a python module or environment
<code>...No such file or directory</code>	You got a path wrong!
<code>slurmstepd:...run-me.py: Permission denied</code>	Your python script doesn't have executable permissions, <code>chmod +x</code> it
<code>bash: cannot set terminal process group (-1)...no job control in this shell</code>	Innocuous error if seen when using <code>srun</code> with a Bash script; ignore
<code>Matplotlib created a temporary config/cache...</code>	Create a directory <code>mkdir .cache</code> in your work directory and add <code>export MPLCONFIGDIR=/work/.../user/.cache/matplotlib</code> to your Bash script before the python command to avoid this warning
<code>slurmstepd: error:...Exec format error</code>	Your python script does not have <code>#!/usr/bin/env python</code> as it's first line
<code>slurmstepd: error: Detected 1 oom-kill event...your job may have been killed by the out-of-memory handler</code>	Your job ran out of memory; increase <code>cpus-per-task</code> in the submission script or write your code in a way to use less memory
<code>I can't (yet) see output from my script in slurm-jobID.out</code>	Cirrus doesn't seem to continuously write output from jobs, so some patience may be required. Adding <code>flush=True</code> to your print statements in python may sort this (otherwise, use the logging module to write messages to a different file entirely).

Table 1: My job won't run!

Common error	Common solutions
WARNING: UNPROTECTED PRIVATE KEY FILE!	The permissions on your private key (the one that doesn't end with .pub) are too lax. From a Linux Shell <code>chmod 600 KEY_FILE</code> will set the right permissions (644 for the public key)
: Permission denied (publickey)	you didn't upload your .pub key to SAFE ; your private/public key pair aren't in the correct place on your system (default <code>~/.ssh/</code> on Linux)
: Broken pipe	Your ssh session timed-out / was interrupted, start a new one
...No entry for terminal type...using DUMB terminal settings...WARNING: terminal is not fully functional	Your terminal emulator is not know/supported by cirrus, setting <code>TERM=xterm-256color</code> before making the connection should be fine in most cases
FILE#-£\$*[NAME]) (: "sad'as#	Stick to using alphanumerical characters and <code>.</code> , <code>-</code> , <code>_</code> in filenames. Using characters that have special meaning in bash e.g. <code>\$</code> , <code>[</code> , <code>?</code> and spaces is bound to result in you having a very bad time when moving files around
something else	Use <code>-v</code> , <code>-vv</code> or <code>-vvv</code> to get verbose output to debug ssh issues

Table 2: Secure shell hell

7 Useful resources

- Cirrus help desk email (monitored Mon–Fri 08:30–18:00): support@cirrus.ac.uk — the service team is typically very quick to respond and helpful (best to contact them using the email associated with your account on [SAFE](#))
- Cirrus documentation, in particular [Connecting to Cirrus](#), [Using Python](#) and [Running Jobs on Cirrus](#).
- [Cirrus Service Status](#) page for live information on all Cirrus subsystems

8 Example files

submit-me.slurm

```
#!/bin/bash

# Slurm job options
#SBATCH --job-name=test-job
#SBATCH --time=96:00:00
#SBATCH --nodes=1           # Leave as 1 to run on same node (each node has 18 cores)
#SBATCH --tasks-per-node=1  # Leave as 1
#SBATCH --cpus-per-task=1   # Leave as 1 unless want multiple cores assigned
#
# Specify project code
#SBATCH --account=d422
# Use the "standard" partition as running on CPU nodes
```

```

#SBATCH --partition=standard
# Use the "standard" QoS as our runtime is less than 4 days
#SBATCH --qos=standard

# Change to a directory under /work - use your own username and desired working directory
cd /work/d422/d422/user/

# Load a relevant python module or environment - uncomment ONE of the following lines
module load python/3.9.13 # System python module, no special environment (set version as required)
#source /work/d422/d422/user/my-env # System python module with environment (edit user/my-env as required)
#source /work/d422/d422/user/miniconda-init.sh; conda activate oqupy # Local Miniconda installation

# Avoid Matplotlib warning
#export MPLCONFIGDIR="/work/d422/d422/user/.cache/matplotlib" # EDIT user

# Launch the job with any arguments passed to this script
srun --cpu-bind=cores ./run-me.py "$@"
# N.B. path is relative to that set by cd above and --cpu-bind=cores option should be used

```

run-me.sh

```

#!/usr/bin/env python

# This script must be executable as user

import sys
print(f"Running {sys.argv[0]} with arguments {sys.argv[1:]}")

```

monitor-memory.sh

```

#!/usr/bin/env bash
# usage:
# ./monitor-memory.sh PID
# where PID is target process
# e.g. monitor memory of most recent srun command:
# srun --cpu-bind=cores run-me.py &
# ./monitor-memory.sh $!
echo $0 "for" $(whoami)"@"$HOSTNAME"
for i in {1..3000}
do
    a=$(date +"%Y-%m-%d %H:%M:%S")
    # rss is resident set size for current shell process
    b=$(ps -o rss= $1 | awk '{printf "%.1f\n", $1 / 1024}') # convert to MB
    if [[ -z "$b" ]]; then
        # if $1 not an existing process, ps returns empty string
        echo "process $1 not found, exiting $0"
        break
    else
        # otherwise print timestamp and memory usage of $1
        echo "$a usage $b MB"
    fi
    # run every minute
    sleep 60
done

```
