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Get Started

Go to ondemand CCR (<https://ondemand.ccr.buffalo.edu>) and login with your UB credentials.
(You can launch batch or interactive apps) BEST BROWSER IS CHROME

Alternative option:

On campus or UB VPN, use secure shell (ssh) -> login node vortex.ccr.buffalo.edu

Preliminary info

- 5 Gb for each user in the home directory
- Up to 1 TB of group space

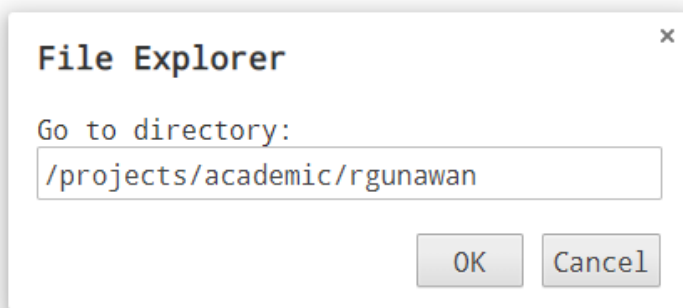
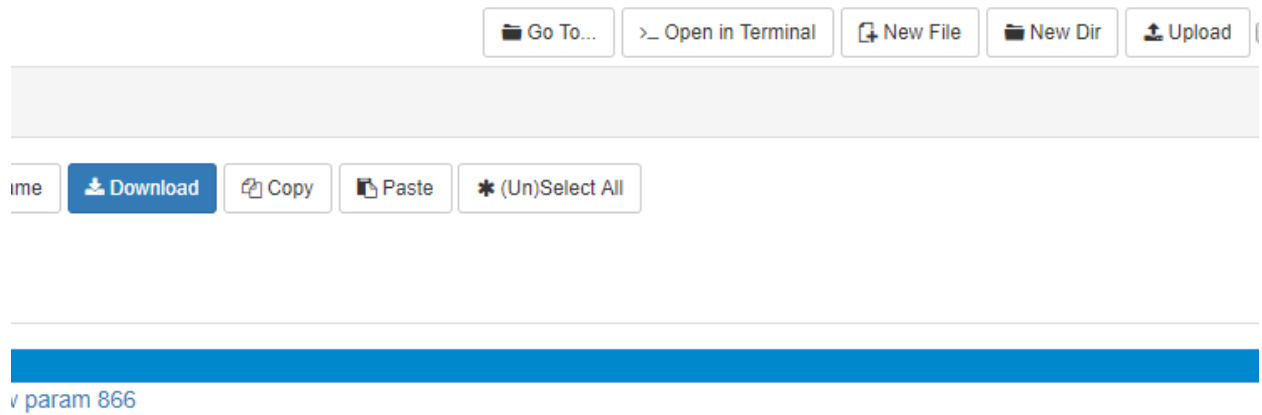
How to transfer files

Files -> home directory -> go to -> /projects/academic/rgunawan and go to single-cell for example

[Files](#) [Jobs](#) [Clusters](#) [Interactive Apps](#) [My Interactive Sessions](#) [Help](#) [Logged in as npgao](#) [Log Out](#)

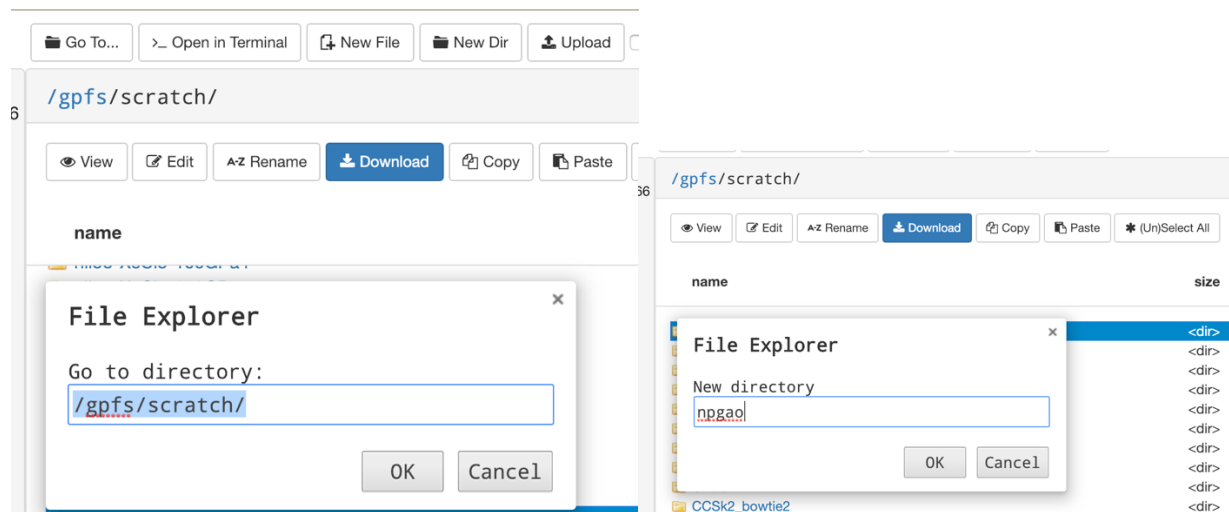
NEW USERS: Please run this script in a terminal window before submitting jobs to the cluster: `/util/ccr/bin/ssh_no_password.sh`

OPEN
OnDemand
OnDemand provides an integrated, single access point for all of your HPC resources.



Create new directory in gpfs/scratch

Goto /gpfs/scratch/ and press “New Dir”



How to install python (or another software) in your own project folder

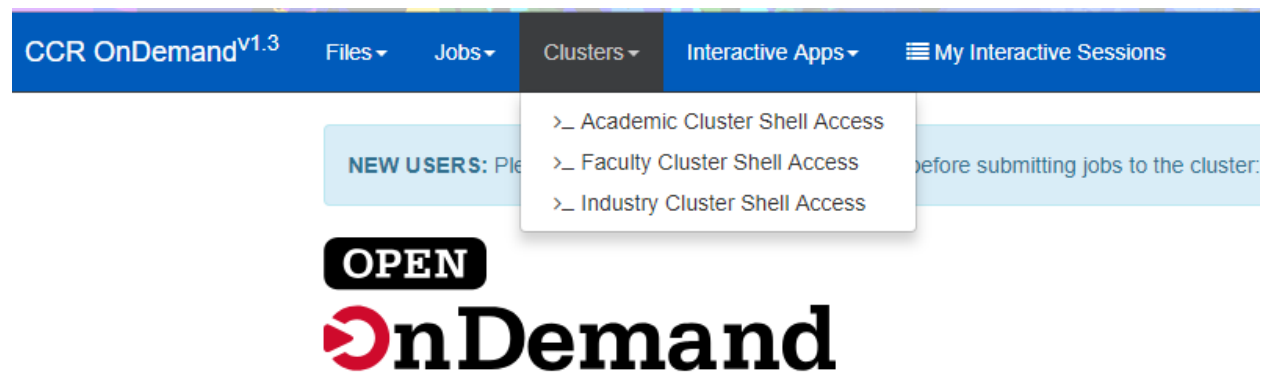
FIRST get the installation file if the version you need is not already available in
/projects/academic/rgunawan/software

OPTION1: download it and transfer to /projects/academic/rgunawan/software/python

OPTION2: “go to” /gpfs/scratch/cdc (FROM CYNTHIA) and copy the file to
/projects/academic/rgunawan/software/python

SECOND

Open terminal from cluster -> academic_cluster_shell..



TYPE:

```
cd /project/academic/rgunawan/software/python/
```

```
ls
```

```
bash Anaconda-2018.12-linux etc.
```

Type yes

Now we are in /user/saberma/anaconda3 then type:

```
/project/academic/rgunawan/software/python/anaconda3-2018.12 for installation
```

Meantime open another window (Open terminal from cluster -> academic_cluster_shell..

```
cd /project/academic/rgunawan/software/python/
```

```
)
```

Type cd /project/academic/rgunawan/software/python/

```
ls -l
```

To see that python is installing!

Then we have to create the module for python:

OPTION2: “go to” /gpfs/scratch/cdc (FROM CYNTHIA) and copy the file to
/projects/academic/rgunawan/module

Now open the file.lua e.g. python37.lua we should type:

```
Whatis([[python37]])
```

Change second line path to :

```
/projects/academic/rgunawan/software/python/Anancona3-2018.02
```

How to load a module:

Make sure the .lua file is present in module directory, i.e.

```
/projects/academic/rgunawan/module/test.lua
```

```
$module avail python
```

```
$module use /projects/academic/rgunawan/module
```

```
$module load test
```

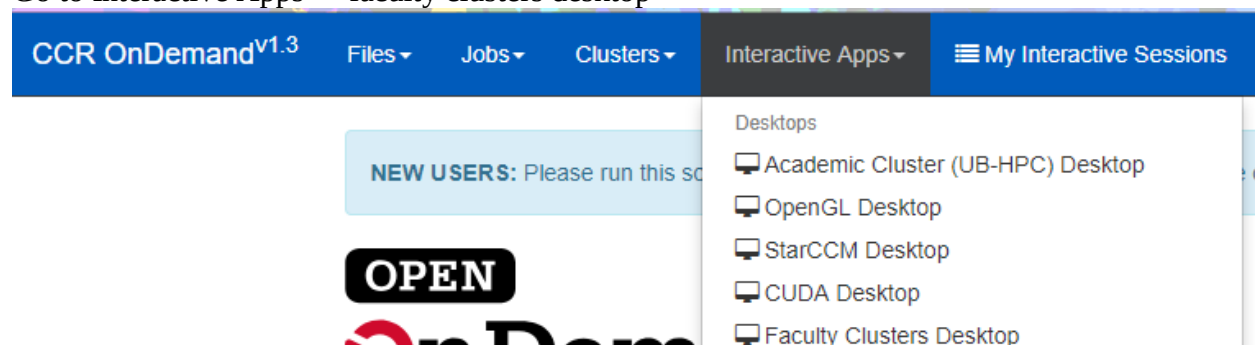
```
$module list (now you should be able to see that your module is loaded)
```

```
$which python (shows your python directory)
```

```
$python -V (shows your python version)
```

How to use our node in interactive mode

Go to Interactive Apps -> faculty clusters desktop



Then enter:

Partition

rgunawan



Please select a partition from the drop-down menu

QOS

rgunawan

Usually the same as partition unless using the 'supporters' QOS on the ub-hpc cluster

Number of hours

1

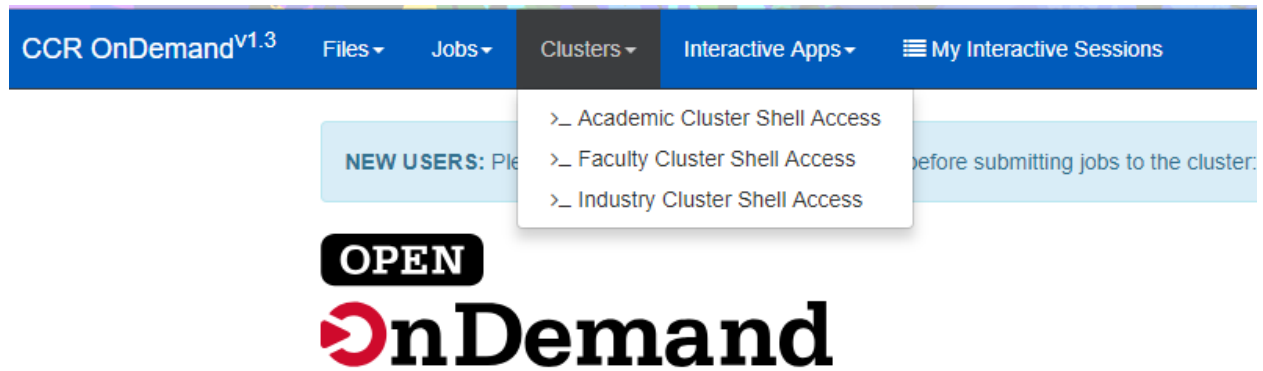
Number of nodes

1

And launch (in interactive sessions we can use only one node).

How to run matlab, rstudio, python

In interactive mode: File system -> File -> open terminal
Otherwise from clusters -> academic cluster shell access



Type:

```
module avail matlab  
module load matlab/R2017b  
matlab -nosoftwareopengl
```

```
module load R  
rstudio
```

(PLEASE TERMINATE YOUR JOB ONCE YOU FINISHED!!!!!!)

Faculty Clusters Desktop (1650886)1 node | 32 cores | Starting

Created at: 2019-02-06 12:58:01 EST

Time Remaining: 1 day

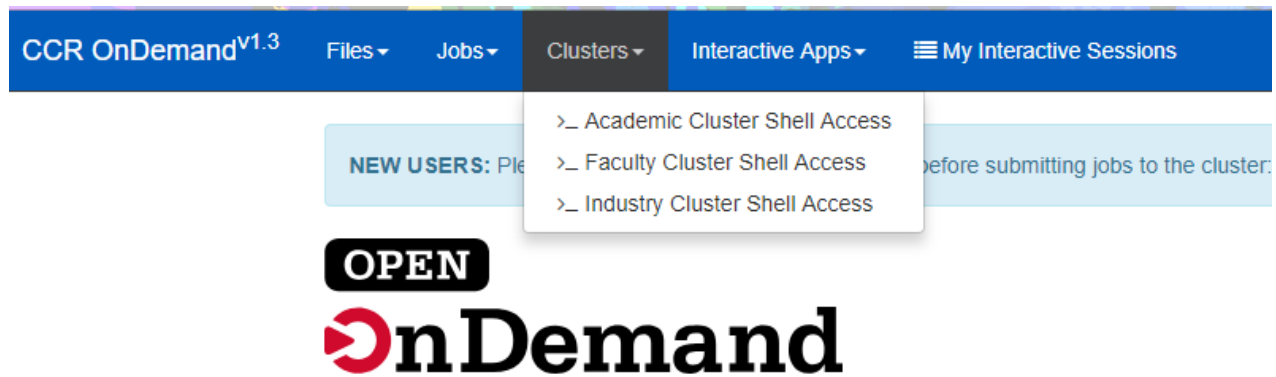
Session ID: 1677732d-ef74-44e0-9721-a2662fce33b2

 Delete

Your session is currently starting... Please be patient as this process can take a few minutes.

How to use cluster and software modules

Go to cluster -> Academic Cluster Shell Access



CCR supports 300+ software packages, installed as modules

module avail (what's installed?)

module load (load modules)

module unload

University at Buffalo The State University of New York

Software Modules

Engineering	Machine Learning	Hadoop/MapReduce	Math/Physics	Image Processing	Utilities
ABAQUS	Caffe	Hadoop	BandUP	EMAN2	7zip
ANSYS	Caffe2	HBase	CrystFEL	FFMPEG	Ant
AVL FIRE	Keras	Hive	FENICS	OpenCV	CMAKE
CFX	MikeNet	Pig	GAP	OpenEXR	DMTCP
COMSOL	TensorFlow	Spark	Gnuid	OpenSlide	gnu-parallel
CPLEX	Theano	ZooKeeper	Gurobi	Environmental	HDF/HDFS
DAKOTA	Torch	GPU Programming	kmos	Cantera	ExchmViewer
Iso2mesh	Data Analytics	CUDA	ROOT	GRASS	Ismi
LSOYNA	edgar	Intel-OpenCL	VMTK	HYSPLIT	Mono
NETGEN	Jags	OpenCL	Visualization	LANDIS-II	netCDF, NCO, CDO
OpenFOAM	MCL	PyCUDA	de.caff	MODFLOW	php2
OpenSees	ms	Editors	NCL	NaSt3DGP	plgr
pyformex	R	Emacs	ParaView	puffin	TauBench
QUCS	SAS	Idle	TecPlot	TELEMAC	tmux
SALOME	Stan	NetBeans	VTK	TITAN	xclip
StarCCM	STATA	Vim	xmgrace	WRF-WPS	xfig

25

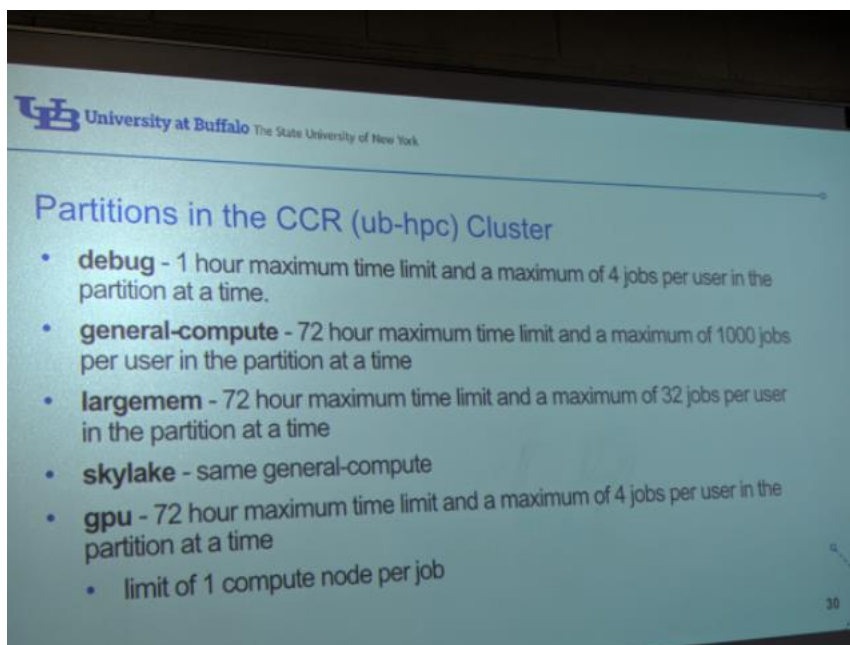
About the Scheduler

SLURM (workload manager)
Useful scheduler commands:

sbatch submit a job script
squeue check the status of a job
scancel delete a job
snodes show node info and status
fisbatch submit an interactive job
salloc request cluster resource for interactive job

Partitions in CCR (ub-hpc) Cluster

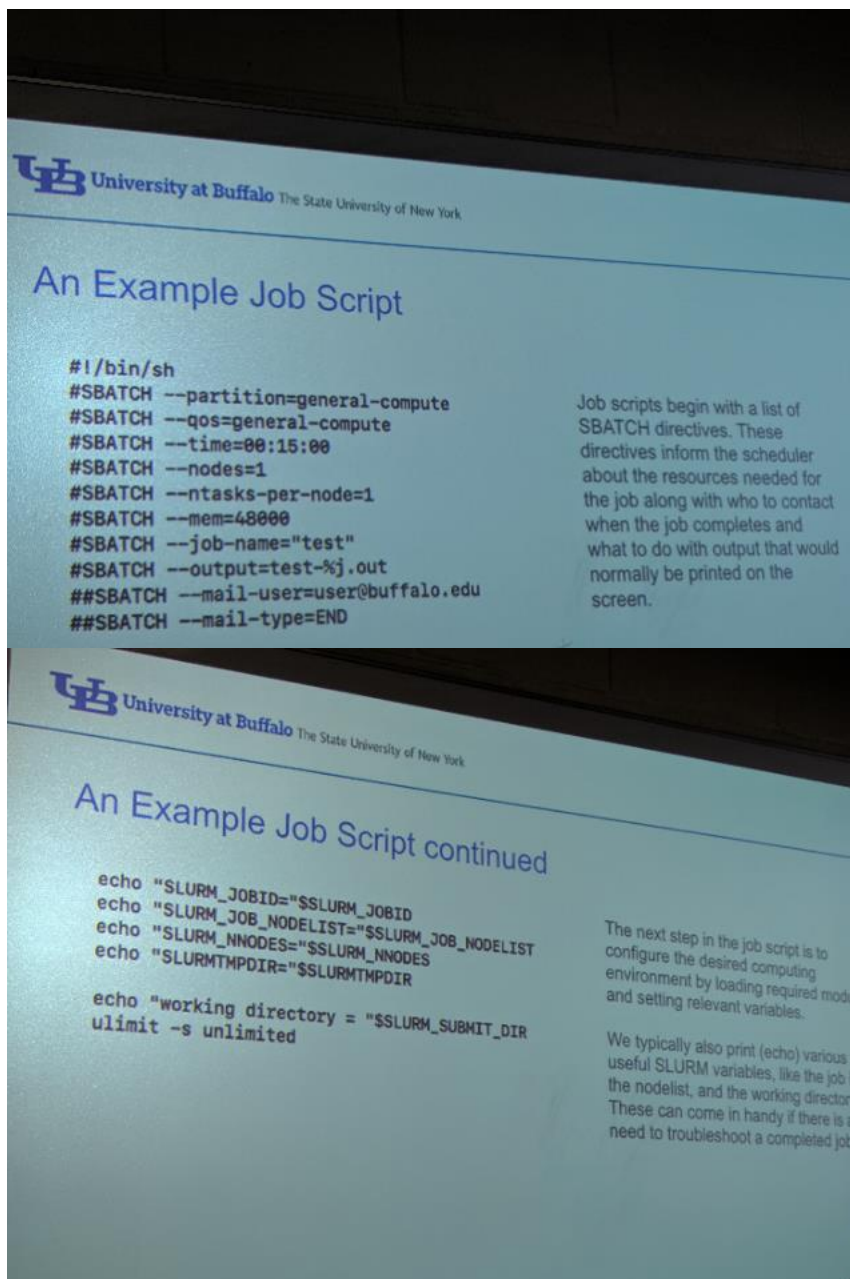
(long story short: skylake is the best one)



NOTE: use the “**snodes**” command to see the details of the compute nodes in partition.

An example job script

Go to the directory of interest to submit the script!



Using faculty partition

slimits to see permissions

sbatch --clusters+mae

squeue -M mae -p rgunawan

snodes all mae/rgunawan to see who's using out nodes

sinfo -M mae -p rgunawan

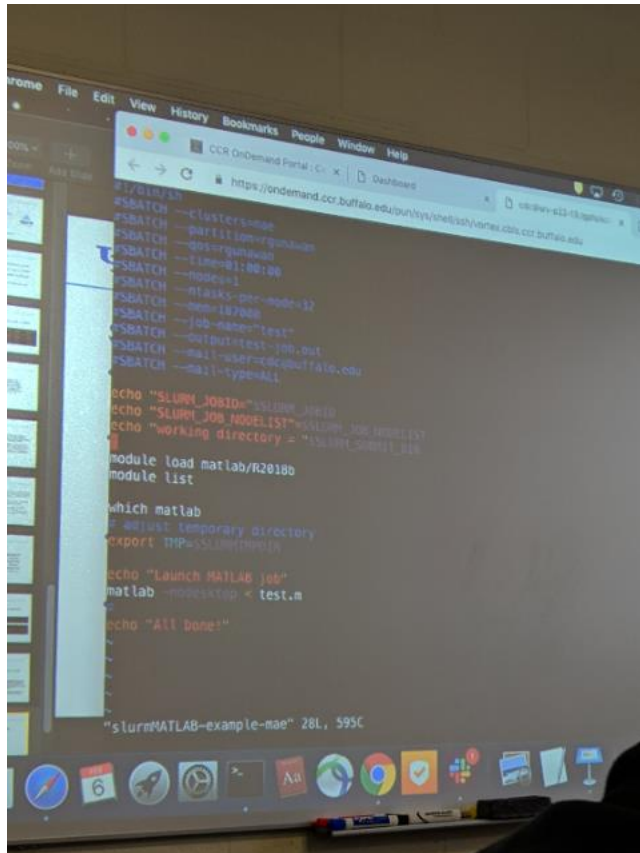
squeue -M mae --nodelist cpn-u12-12 to see the scavenger muahahah

sinfo -M mae -p rgunawan

Practical example of running MATLAB script

```
cd /gpfs/scratch/cdc
```

copy the entire folder matlab-example in your home
modify slurmMATLAB-example-mae



Cd to the matlab-example folder in you directory.

```
cd ./matlab-example
```

Now run it on the terminal with : **sbatch slurmMATLAB-example-mae**

```
[npgao@vortex1:~/matlab-example]$ sbatch slurmMATLAB-example-mae
Submitted batch job 1650996 on cluster mae
[npgao@vortex1:~/matlab-example]$ squeue -M mae -p rgunawan
CLUSTER: mae
      JOBID PARTITION    NAME     USER ST       TIME  NODES NODELIST(REASON)
      1650996 rgunawan    test      npgao R        0:41       1 cpn-u12-11
[npgao@vortex1:~/matlab-example]$ ssh cpn-u12-11
```

more test.m (check matlab file)

more test-job.out

How to load and use Tigramite package

Start an interactive session on OnDemand and open Terminal.

```
$module use /projects/academic/rgunawan/module
```

```
$module load tigramite (or tigramite-parallel in case you want to run in parallel)
```

```
$export XDG_RUNTIME_DIR=/projects/academic/rgunawan/scratch
```

```
$spyder
```