

Oscar: Sage

Loading and Launching Sage

1. Once authenticated to Oscar, use the following commands at the command line.
2. Start an interactive job by using the `interact` command. This command can take additional parameters to extend the resources and time allotted to the node as well as the partition that the node operates on.
3. The Sage module provides containers. To load them, use `module load sage-container/10.3`.
4. To start the container, use `apptainer shell /oscar/rt/9.2/software/0.20-generic/0.20.1/opt/spack/linux-rhel9-x86_64_v3/gcc-11.3.1/sage-container-10.3-avpqi pfsnbneig726l72jrgdmlrivg4m/sage.sif`
5. Once inside the container's shell, use `sage` to launch the Sage console.

Sage on Oscar OnDemand

The easiest way to run Sage on Oscar OcDemand is to run sage in an interactive job via the terminal in your OnDemand session.

Use the `interact` command with parameters for your specific job to start the interactive session, then load your modules and run the sage binary (steps 2-4 above).

```
interact -n 2 -m 32g -t 04:00:00 -f 'haswell|broadwell|skylake'
```

Using Sage with Batch Scripts

Thanks to Trevor Hyde from Summer@ICERM 2019 for these instructions.

One method for running computations with Sage on Oscar is to write a script and use the slurm batch scheduler to have Oscar run your script. This requires two pieces:

1. A shell script to configure and submit your batch job to the cluster.
2. Your Sage code/program you'd like to run.

Example Batch Script

sage-batch.sh

```
#!/bin/bash

#SBATCH -J test_program
#SBATCH --array=0-9
#SBATCH -t 1:00:00
#SBATCH --mem=8G

#SBATCH -e data/<oscar-username>/test_output/test%a.err
#SBATCH -o data/<oscar-username>/test_output/test%a.out

module load sage-container/10.3

apptainer shell /oscar/rt/9.2/software/0.20-generic/0.20.1/opt/spack/linux-rhel9-x86_64_v3/gcc-11.3.1/sage-
container-10.3-avpqipfsnbneig726l72jrgdmlrivg4m/sage.sif

sage test_program.sage $SLURM_ARRAY_TASK_ID
```

- `#!/bin/bash` tells the system this is a bash (shell) script.
- `#SBATCH -J test_program` sets the name of the job which appears when you check the status of your jobs.
- `#SBATCH --array=0-9` is an easy way of doing parallel computations. In this case it says our job will run on 10 different nodes, each node will be passed a parameter and we have specified that the parameters will take the values 0 through 9. You can specify several ranges or even list individual parameters if you prefer.
- `#SBATCH -t 1:00:00` specifies a time limit in `HH:MM:SS` for each node. Once this time runs out your program will stop running on that node. Be careful setting the time limit too high as doing so may make it take a long time for your job to get scheduled to run. Before starting a big computation try to do some smaller tests to see how long you expect to need.
- `#SBATCH --mem=8G` specifies how much memory each node gets. Standard exploratory accounts get 123GB total to use at any one time. So if you allocate too much per job, fewer jobs will run at once. On the other hand, if you allocate too little and a computation needs more than it has, then it will terminate. If this happens an “out of memory” error will show up in the `.err` file for that node.

- `#SBATCH -e data/<ccv-username>/test_output/test%a.err` and `#SBATCH -o data/<ccv-username>/test_output/test%a.out` specify where the error messages and output for each computation should be sent. You should store these files in your user folder, not on the submit node. We each have a folder inside the `data` directory which you can see from the submit node. In this example I have created a folder titled `test_output` where I'm putting both of these files. **You need to make these folders before you run the computation otherwise the output will be dumped into the void!** The `%a` will get replaced with the array parameter. So for example, since we set our array parameters to be `0-9` there will be 10 nodes running and each of them gets a number between 0 and 9; this node corresponding to the parameter 7 will create two files `test7.err` and `test7.out`.
- `module load sage-container/10.3` loads the sage container into the node.
- `apptainer shell /oscar/rt/9.2/software/0.20-generic/0.20.1/opt/spack/linux-rhel9-x86_64_v3/gcc-11.3.1/sage-container-10.3-avpqi pfsnbneig726l72jrgdmlrivg4m/sage.sif` initiates the container's Sage console shell.

Everything after this in the script happens as if you typed it yourself onto the command line.

- In our example, we want to run sage code, so the line `sage test_program.sage` `$SLURM_ARRAY_TASK_ID` runs our example sage program `test_program.sage`.
- The file needs to have the `.sage` extension.
- You should write this file in a text editor, not in a Jupyter notebook (although you can first write and test your program in a Jupyter notebook and then copy and paste it into a new file when it's ready).
- This program is written to accept one input and I have passed it `$SLURM_ARRAY_TASK_ID` which is the array parameter passed to each node. You can use this parameter to select which input parameters to run your program on.

Example Sage Program

`test_program.sage`

```
import sys

def fun_math(message):
    print message
    sys.stdout.flush()

job_id = int(sys.argv[1])
fun_math('hi this is a test')
fun_math('my job id is' + str(job_id))
```

- In the Sage program, you first define all of your functions and then you include the code you want to run.

- Import `sys` so you can access the array parameter passed to your function from the node. This is accessed in this case by `sys.argv[1]`. Make sure you explicitly coerce to be an integer if you want to use it as an integer; it's a string by default.
- The output of the `print` command is appended to the `.out` file for this node as a new line.
- Notice the line `sys.stdout.flush()` included in the function. This makes the program immediately send whatever output it has to the output file when called. Otherwise the program won't output **anything** until it has completely finished running. If each node is running 100 potentially long computations and it finishes the first 99 but then times out on the 100th computation, and you don't include any `sys.stdout.flush()` commands, everything will be lost when time runs out.

Submitting the Batch Job

- To run this batch program go back to the submit node and type `sbatch <NAME_OF_BATCH_FILE>`. In our example here, our batch file is called `sage-batch.sh`, so we simply type `sbatch sage-batch.sh`. Slurm will return a line that tells you your job has been submitted together with a job id number.
- To check the progress of your jobs type `myq` from anywhere on Oscar. This will show you what jobs you have running, how much time they have left, and which jobs are still waiting to run. Be patient, sometimes it takes a minute for things to get started.
- If you realize your code is never going to finish or that you've made some terrible mistake, you can cancel a batch job by typing `scancel <JOB_ID>`. You can specify a single node or just put the general job id for the whole run and cancel everything.

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