Created cluster

Create database

Add ip address

Choose connection method – change driver to correct python version, then get the connection string

Need to add the IP addresses to the whitelisted addresses on the supercomputer – if you click inside your specific cluster (defaults to cluster0), three nodes will show up – two secondary and one primary. You just need to copy those and delete the :27017 from the end, and those are the three sites that need to get approved.

This is meant as a supplement to the instructions found on the Atomate Installation page, based on errors I encountered and ways that I found around them. Some of these errors may have been unique to me, as I am not yet an experienced programmer. I will provide the final setup of my files at the end.

1. **Virtual Env - Modules:**
   1. Instead of using the default modules on the supercomputer, purge the modules and then load python/3.8 and gcc/9 before creating the virtual environment for Atomate (you can run “module list” to see which modules are currently installed, “module purge” to remove them, “module avail” to see which ones are available, and then “module load <<module\_name>>” to load new ones)
2. Pip install the maggma package – it is a dependent package that does not get downloaded as part of atomate.
3. **Db.json file**:
   1. The port is just 27017
   2. Add the following line to the end "authsource":"admin"
   3. The hostname can be somewhat particular, it should be of the form "host":"mongodb+srv://cluster0.9esxz.mongodb.net." You may need to delete some stuff in the middle. You can find the name of the host if you go on the mongodb website, then under Clusters, click on Connect for the cluster you would like to connect to, then for “Choose a connection method” select “Connect your application,” then select Python under the driver and the whatever version you are using. For me, that generated a line “mongodb+srv://<username>:<password>@cluster0.9esxz.mongodb.net/myFirstDatabase?retryWrites=true&w=majority,” which I deleted stuff from until it was simply “mongodb+srv://cluster0.9esxz.mongodb.net."
      1. I found this explanation on another site: Use this connection string format: mongodb+srv://:@<cluster\_name>.mongodb.net/. If you have a cluster's connection string with servers' names like: cluster0-\_shard-00-00-\_jxeqq.mongodb.net, modify your server's name by removing shards' info so your <cluster\_name> looks like this:cluster0-jxeqq.mongodb.net
   4. NOTE: The system administrators for the supercomputer will have to add the IP address of the cluster to their whitelist in order for it to connect while running jobs
4. **My\_fireworker.yaml**
   1. The vasp\_cmd line was somewhat confusing. What ended up working was providing the path to the executable for vasp, which in my case was /fslhome/glh43/fsl\_groups/fslg\_msg\_code/bin/vasp6\_mpi. Consequently, that line is NOT needed in the my\_qadapter.yaml file, or in the template file if you choose to set one of those up.
5. **My\_launchpad.yaml**
   1. Add the following two lines to the end:
      1. ssl: True
      2. authsource: admin
   2. If you don’t, you will likely get a connection error that says “pymongo.errors.ServerSelectionTimeoutError: connection closed”
6. **My\_qadapter.yaml**
   1. The default file in the installation tutorial does not contain the amount of memory requested per cpu, which is a requirement for submission on the BYU system (and it also may have needed ntasks and nodes).
   2. One way to get around that is to add the SLURM\_template.txt to your config directory, reference it as a template, and then add the information for the memory per cpu. The SLURM\_template.txt can copied from Github: <https://github.com/materialsproject/fireworks/blob/main/fireworks/user_objects/queue_adapters/SLURM_template.txt>
   3. For further clarification, see the full text below.
   4. The exact specifications for the runs may depend on the size of job you are using, but I have found using “nodes: 1,” “ntasks: 2,” “mem-per-cpu: 10G,” and “walltime: 24:00:00” to provide enough wiggle room in memory to prevent crashes
7. **Pymatgen and Potcars**: I recommend viewing the pymatgen instructions at <https://pymatgen.org/installation.html#potcar-setup> , which are more detailed than those at on the atomate website. Note: if you copy the potpaw\_PBE file, you will have to run the "pmg config" command on the directory ABOVE potpaw\_PBE, or it won't do it properly. For example, if you copy the potpaw\_PBE folder in a folder called potcarTempStorage, you would run "pmg config -p potcarTempStorage <MY\_PSP>"
8. **Materials API Key:** See the following instructions from the bottom of the pymatgen docs Usage section: <https://pymatgen.org/usage.html#setting-the-pmg-mapi-key-in-the-config-file> This personal key can be generated on the Materials project website.
9. **Bash Profile:**
   1. If you don’t have one already, in your home directory create a file “.bash\_profile”
   2. Add “ulimit -s unlimited” to it – that prevents VASP from having segmentation errors
   3. Also add “export FW\_CONFIG\_FILE=/<path>/atomate/config/FW\_config.yaml,” or you will get connection errors with the mongo database
10. **[Errno 101] Network is unreachable**:
    1. If you are getting this in the FW\_job<<number>>.error file, then the system administrators have not yet enabled access to the cloud database – see the db.json section

**Full text for Files:**

I highlighted lines that are added or altered from those suggested in the installation guide. Also, if anyone is like me and did not understand the <<>> notation, it indicates a substitution, and you remove it when you add your info – for example, if your database is called atomate\_database, then "<<database\_name>>" becomes “atomate\_database.”

**Db.json**

{

"host":"mongodb+srv://cluster0.9esxz.mongodb.net",

"port":27017,

"database":"<<database\_name>>",

"collection":"<<collection\_name>>",

"admin\_user":"<<admin\_username>>",

"admin\_password":"<<admin\_password>>",

"readonly\_user":"<<read\_user\_name>>",

"readonly\_password":"<<user\_password>>",

"aliases":{},

"authsource":"admin"

}

**My\_fireworker.yaml:**

name: <<worker\_name>>

category: ''

query: '{}'

env:

db\_file: /<<path>>/atomate/config/db.json

vasp\_cmd: /fslhome/glh43/fsl\_groups/fslg\_msg\_code/bin/vasp6\_mpi

scratch\_dir: null

**My\_launchpad.yaml:**

host: mongodb+srv://cluster0.9esxz.mongodb.net

port: 27017

name: <<database\_name>>

username: <<admin\_username>>

password: <<admin\_password>>

ssl\_ca\_file: null

logdir: null

strm\_lvl: INFO

user\_indices: []

wf\_user\_indices: []

ssl: True

authsource: admin

**My\_qadapter.yaml:**

\_fw\_name: CommonAdapter

\_fw\_q\_type: SLURM

\_fw\_template\_file: /<<path>>/atomate/config/SLURM\_template.txt

rocket\_launch: rlaunch -c /<<path>>/atomate/config rapidfire

nodes: 1

ntasks: 2

mem\_per\_cpu: 10G

walltime: 24:00:00

queue: null

account: null

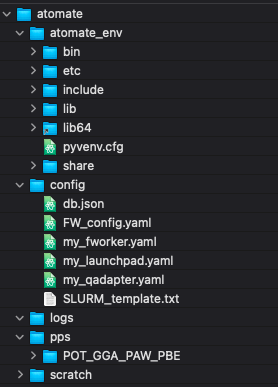
job\_name: null

pre\_rocket: null

post\_rocket: null

logdir: /<<path>>/atomate/logs

The final file structure should look like the following:



{

"host":"mongodb+srv://cluster0.9esxz.mongodb.net",

"port":27017,

"database":"introproj",

"collection":"tasks",

"admin\_user":"calebcsjm",

"admin\_password":"mimamima1",

"readonly\_user":"readuser",

"readonly\_password":"mimamima1",

"aliases":{},

"authsource":"admin"

}

[cluster0-shard-00-01.9esxz.mongodb.net](https://cloud.mongodb.com/v2/603f2804ac11b6401f5e4218#metrics/host/3d25d517f4c349b010408992d70e91e3/status)

[cluster0-shard-00-02.9esxz.mongodb.net:27017](https://cloud.mongodb.com/v2/603f2804ac11b6401f5e4218#metrics/host/dbf99011af980b537ab62656bd2f8bd8/status)

Other edits to the source code:

* Turning off the max\_force\_threshold, since that causes some things to quit
  + atomate/vasp/fireworks/core.py, OptimizeFW, line 68
  + See <https://matsci.org/t/maxforceerrorhandler/4414>