

Usage:

preparation at kugui

We use kugui. (or ucgw in osaka-u)

At kugui set following lines at .bashrc.

```
if [ -z "$PS1" ]; then
    source /etc/profile.d/modules.sh
fi
export PATH=/opt/pbs/bin/:$PATH
```

usage

```
cp -r testSGA0/ testSGA #note testSGA is empty
./jobtestSGA #look into jobtestSGA.
```

Mechanism memo. How it works.

See jobautoplan.md.

0. starting.

We have initial testSGA0/ as

```
testSGA/
├─ init
│   ├── POSCARALL
│   │   ├── POSCAR.mp-1330
│   │   └── POSCAR.mp-149
│   │   ...
│   ├── qsub.0          :qsub template
└─ qsub.dependency.0    :dependency fileempty, always)
```

1. initial set up stage

Take a look at testSGA0/. We have testSGW0/init/qsub.0, which is a template of qsub. testSGW0/init/qsub.0 is machine-independent. Note variables `__foobar__` in it.

`__foobar__` are replaced by the arguments given to `jobmon.py`.

At first, we do `cp -r testSGA0/ at testSGA/` (note: we need testSGA0/==testSGA/. Careful when testSGA/ already).

Then we apply `python initposcar.py --ldir=testSGA` at the beginnig of jobtestSGA.

This just initialize the directory of testSGA/

That is, to distribute qsub.0, qsub.dependency.0, and POSCARALL/POSCAR* under testSGA/*

After `python initposcar.py --ldir=testSGA'`, we have directories as

```
testSGA/
├── ...
│   ├── mp-1330
│   │   ├── POSCAR.mp-1330
│   │   ├── qsub.0
│   │   └── qsub.dependency.0
│   └── ...
```

2. The second step of ./jobtestSGA

This is the main part of job control. See the bottom of jobtestSGA, where we run

```
python auto/jobmon.py --user k041303 --remote kugui --
pythonpath=/home/k0413/k041303/.local/share/mise/installs/python/3.13.0/
bin/python --binpath=/home/k0413/k041303/bin --ldir=testSGA --
rdir=/home/k0413/k041303/testSGA111 --maxqsub=3 --maxcore=4 --quiet --
qsubheader=qsubheader.kugui2.temp --qstatcommand='qstat '
```

(note: `python auto/jobmon.py --help` gives a help).

- `qsubheader.kugui2.temp` is given by Here Document in jobtestSGA. We need another here documents for other machine, and set `--qsubheader=qsubheader.kugui2.temp`).