

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

At ecalj/jobauto/, run **>tree testSGA**.

Then you see init0/ directory.

qsub.0 is default qsub script.

All POSCAR is under POSCARALL/

Run

```
> ./jobtestSGA
```

Look into the bash script **jobtestSGA**.

You have to customize this for your purpose.

Mechanism memo. How it works.

0. starting.

PROF

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

- We have testSGW/init0/qsub.0, which is a template of qsub. testSGW/init/qsub.0 is not machine-dependent. `__foobar__` are replaced with the augments given to `jobmon.py`. See `jobtestSGA`.
- We apply `python initposcar.py --ldir=testSGA` at the beginning of `jobtestSGA`. This creates the directory `testSGA/init` from `init0/`. `initposcar.py` distributes `qsub.0`, `qsub.dependency.0`, and `POSCARALL/POSCAR*` under `testSGA/mp*`

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

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

2. The main step of `./jobtestSGA`

See the bottom of `jobtestSGA`, where we run

```
python auto/jobmon.py --user k041303 --remote kugui --pythonpath=...'
```

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

- `qsubheader.kugui2.temp` is given by the Here Document in `jobtestSGA`. We include machine-dependent here documents in it. Set `--qsubheader=qsubheader.kugui2.temp` to specify which one.
- See [the algorism of jobmon.py](#)