

# Jacapo

## Submitting Batch Jobs

```
jacapo-bsub myscript.py
jacapo-ver-bsub 9a myscript.py (select a specific version)
```

## Jacapo Parallel NEB Example

You can find a Jacapo parallel NEB example [here](#). This same script can be used for a restart (the interpolated traj files are only recreated if they don't exist).

Some important notes:

- the number of processors selected for a parallel NEB must be an integer multiple of the NumberOfImages-2 (the images at the end points are "fixed").
- Parallel NEB settings (e.g. number of cores) can be debugged running in the suncat-test queue with 1 processor per non-fixed image.
- Later on in the NEB (discussed [here](#)) it is good to set climbing=True and switch to the FIRE method, shown [here](#). As best I can tell, this page doesn't provide good instructions for when to turn those on.

## Perturbing Jacapo Calculations

When taking an existing Jacapo calculation and making changes (e.g. adding an external field) it is important to not instantiate a new calculator (to work around some Jacapo bugs) but instead read in the previous atoms/calculator from the .nc file. Johannes Voss has kindly provided an example with some comments [here](#).

## Stripping Wavefunctions from Jacapo .nc Files

To strip wavefunctions from all subdirectories of the current directory (".", in the find command):

```
source /afs/slac/g/suncat/jacapo/setupenv
find . -name \*nc -exec /nfs/slac/g/suncatfs/sw/jacapov3/ase/ase/calculators/jacapo/tools/stripnetcdf {} \; -
print
```

## Versions

Version	Date	Comment
jacapov3	4/29/11	copy of v2, but ase from svn head to pick up Lars parallel neb code (and dacapo.run)
jacapov4	7/8/11	softlink to jacapov3, change setupenv/dacapo.run to use torque/maui aware openmpi
jacapov5	2/23/12	softlink to javapov3, change setupenv/dacapo.run to use lcls filesystem naming /reg/d/suncat
jacapov6	3/7/12	like v5, but use the TaskStarter/mympirun_wrapper script in dacapo.run so we can bstop/bresume jobs and fix accounting for non parneb jobs
jacapov7	4/12/12	like v6, but change dacapo.run script so that it can be used for normal jobs and parallel nebs
jacapov8	11/5/12	like v7, but change dacapo.run script to not use /afs version of mpirun. Appears to fix intermittent hang problem with parallel NEBs
jacapov9a	11/9/12	(suncat3 farm only) python packages rebuilt for RHEL6
jacapov10	2/21/13	like v8, but more recent version of ASE (3.6.1.2694)