

# 1 AFLOW $\pi$ Configuration file

Variable Name	Type	Description	Req?
work_dir	Text	Path of the directory where AFLOW $\pi$ will generate the directory tree. Typically this path will be in a scratch partition.	Y
pseudo_dir	Text	Path of the directory containing the pseudopotential files you want to use in your calculations	Y
engine_dir	Text	Path of the directory containing the executables of your calculation engine	Y
gipaw_dir	Text	Path of the directory containing the executables. Required if workflow contains steps that use GIPAW.	D
pao_dir	Text	Path of the directory containing the gaussian basis files used in ACBN0. Required if workflow contains ACBN0.	D
fig_dir	Text	Path of directory where figures will be copied to. If omitted, figures will only be generated in the directory tree.	N
engine	Text	Type of calculation engine. Only engine currently supported is Quantum Espresso	N
exec_prefix	Text	Runtime execution prefix. ex. mpirun -n 64	N
exec_postfix	Text	Runtime execution postfix. ex. -npool 4	N
exec_prefix_serial	Text	Overrides exec_postfix for serial executables. On some computing clusters certain executables do not run properly with parallel execution prefixes	N
exec_postfix_serial	Text	Overrides exec_postfix for serial executables. When using exec_prefix_serial it is sometimes necessary to also override the exec_postfix	N
exec_postfix_nscf	Text	Overrides exec_postfix for the nscf step of ACBN0 or the generation of PAO-TB hamiltonians	N
queue	Text	Name of queue to send PBS jobs to. On some cluster computers this is needed. -q value is appended to the qsub command.	D
job_template	Text	Path of the cluster job submission template. Required if submitting calculations to a queue.	D
steps_as_jobs	Bool	If True: Each step in the calculation workflow will be submitted as a new job. Can be useful in certain situations like a very long workflow.	N
restart_buffer	Float	Amount of buffer time to include in diring the runtime of the workflow. The buffer allows the calculation engine to gracefully exit before hitting the walltime requested for the cluster job. The job will automatically resubmit itself and restart where it left off. If the value is less than 1.0 then it the buffer will be a (1-value)*walltime requested for the job. If the value is greater than 1.0 then the buffer will be that number of seconds. Default is 0.9	N

Variable Name	Type	Description	Req?
cluster_type	Text	Type of cluster submission/queue system. Required if submitting jobs to a queue. if not included the calculations will run locally.	D
author	Text	Name of user	N
affiliation	Text	Affiliation of user	
title	Text	Title of project	N
log_level	Text	Logging level of AFLOW $\pi$ . Acceptable values: CRITICAL, ERROR, WARNING, INFO, DEBUG. Default is INFO	N
plot_file_type	Text	File extension of generated figures. Acceptable values: .png and .pdf. default is .png.	N
pseudo_regex	Text	Custom regular expression used to choose a pseudopotential file from pseudo_dir. Rarely needed.	N
copy_execs	Bool	Whether to copy executables to the directory tree or use symbolic links instead. Default is True	N
copy_pseudos	Bool	Whether to copy pseudopotentials to the directory tree or use symbolic links instead. Default is True	N