

Minner

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Minner can minimize the energy over an arbitrary set of variables or create data sets for an arbitrary set of variables.

New:

there is a config directory `$HOME/.minner`, which contains the file `default`, which allows to set a default run environment, which gets used when new a `=.min` file is created by minner (if run in a directory not containing `=.min`). On a fresh start of minner this file gets created, if not already existing. Same for `$HOME/.minner/pbs/pbs.sh`, which gets created on the first run of minner. This file can be edited and contains placeholders marked by `%%`, example: `%mem%`. These placeholders are filled by minner with the actual settings contained in `=.min`. The user can adapt `$HOME/.minner/pbs/pbs.sh` to his/her needs, according to the local pbs system specifications.

The run environment is explained in the following. Note, that some of these variables are only used in the `pbs.sh` batch script. Here we only explain what they are ment to be used for. Currently a pbs batch system for job submission is assumed to be present in your cluster.

fplo This must hold the full path to the fplo executable used for input creation. Normally, this is the one running on the job submission machine.

runfplo This must hold the full path of the executable used on the calculation node. The path must be valid when the job is actually running on the node.

fedit This must hold the full path to the fedit executable used for input creation. Normally, this is the one running on the job submission machine.

method default: PBS. This is the name of the batch system used for job submission. Note, that modern Linux systems offer torque, which is a pbs system. Consult your system administrator to set it up, or use google to set it up yourself.

forceinitialspinsplit **f** or **t**: if **f** (false) the initial spin split question of fplo is answered such that the split is avoided. If **t** the split is enforced. Of course only if the fedit input requests such a split.

forceconvergence: **f** or **t**: currently not used.

copydata: **f** or **t**: if the default pbs.sh script is used, it can either copy data to the remote calculation node or it cannot. You copy when the node's file system is different from the submission machine's file system. You do not copy, if the nodes and the submission machines file system are the same. Note, that if copy is needed in general, copying is avoided, if the submission machine equals the calculation node.

deleteonnode: **f** or **t**: If copying is done, the data are copied back from the calculation node to the submission machine. After this is done the data on the calculation node are deleted if this option is **t**.

time: 01:00:00, the allocated maximum time for the calculations.

memory: 500mb, the allocated maximum memeory for the calculations.

name: a job name. (The same for all minner jobs.)