

Environment Variables

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To compile PSCF+ in a Unix environment, before compiling any code, the user should modify the following Unix environment variables:

- Add the `pscfplus/bin/` directory to the Unix `$PATH` shell environment variable (the shell command search path). By default, executable file created by the PSCF+ build system is installed in the `pscfplus/bin/` directory. The directory in which these files are located must be added to the user's `$PATH` variable in order to allow the Unix shell to find the executable file when it is invoked by name in a command executed from any other directory.
- Add the `pscfplus/lib/python` directory to the `$PYTHONPATH` environment variable (the python module search path). The `pscfplus/scripts/python` directory contains a python script that is used by the build system during compilation to generate information about dependencies among C++ files. This directory must be added to the `$PYTHONPATH` variable in order to allow the python interpreter to find this file.

To make these changes using a bash shell, add some variant of the following lines to the `.profile` or `.bash_profile` file in your user home directory:

```
PSCFPLUS_DIR=${HOME}/pscfplus
export PATH=${PATH}:${PSCFPLUS_DIR}/bin
export PYTHONPATH=${PYTHONPATH}:${PSCFPLUS_DIR}/scripts/python
```

The value of `PSCFPLUS_DIR` should be set to the path to the PSCF+ root directory (*i.e.*, the root of the directory tree created by cloning the PSCF+ git repository). In the above fragment, as an example, it is assumed that this is a subdirectory named `pscfplus/` within the user's home directory.

After adding an appropriate variant of these lines to `.profile` or `.bash_profile`, re-login, and then enter `echo $PATH` and `echo $PYTHONPATH` to make sure that these variables have been set correctly.

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