Compilation

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Below are the instructions for compiling the PSCF+ program with examples. It is assumed that you have cloned the PSCF+ repository and installed all required dependencies, and that the root directory of the repository is named `pscfplus/`.

Instructions:

- **Set environment variables:** Modify the user's $PATH and $PYTHONPATH Unix environment variables, as discussed **here**.
- **Navigate to root directory:** Change directory (`cd`) to the `pscfplus/` root directory.
- **Setup:** Invoke the "setup" script from the `pscfplus/` root directory. Enter the command

  ```
  > ./setup
  ```

  to setup the build system with default compiler options. Alternatively, invoke the setup with a filename argument for non-default compiler options.
- **Change directory to the build directory:** Change directory (`cd`) to the `pscfplus/bld` subdirectory, by entering `cd bld` from the root directory.
- **Compile the PSCF+ program for a given model system:** From `pscflus/bld`, enter

  ```
  > bash compile.sh [-B CHN] [-N NBP] [-C] [-D] [-K K]
  ```

  This will generate a large number of intermediate object (`*.o`), dependency (`*.d`) and library (`*.a`) files in subdirectories of the `pscfplus/bld` directory, and install the executables in the `pscfplus/bin` directory. The options in the above command are as follows:
  - CHN: Specifying the model of chain connectivity (by default it is the continuous Gaussian chain); see Models.pdf for details.

    ```
    DGC: discrete Gaussian chain
    FJC: freely jointed chain
    ```
  - NBP: Specifying the form of non-bonded pair potential (by default it is the Dirac δ-function potential); see Models.pdf for details.

    ```
    G: Gaussian potential
    DPD: dissipative particle dynamics potential
    SS: soft-sphere potential
    ```
  - `-C`: Specifying a compressible system (by default the system is incompressible); see Models.pdf for details.
  - `-D`: Specifying the use of discrete cosine transforms between the real and reciprocal space (by default the fast Fourier transforms are used.)
  - `-K`: Specifying the *K*-value of the REPS-*K* method (by default the REPS-1 method is used); this is used only for the continuous-Gaussian-chain models (see REPS.pdf for details.)

Examples:

- **Compilation for the "standard" model:** To compile PSCF+ for calculations of the “standard” model (*i.e.*, incompressible melts of continuous Gaussian chains with the Dirac δ-function repulsion) using the REPS-1

method and fast Fourier transforms (same as used in PSCF), simply use the following command:

```
bash compile.sh
```

- **Compilation for the DPDC model:** To compile PSCF+ for calculations of the DPDC model (*i.e.*, compressible melts of discrete Gaussian chains with the dissipative particle dynamics potential) using fast Fourier transforms, users can use the following command:

```
bash compile.sh -B DGC -C -N DPD
```

- To get a list of the aboved options, use the following command:

```
bash compile.sh -h
```