Invoking an Executable

Calculation of a single (ordered) phase

Here is an example of command-line usage of PSCF+ program for calculation of a single ordered phase:

```
pg [-e] -d D
```

In the above, `pg` is the name of executable, `-e` activates echoing of the parameter file to standard output (which is optional), dimensionality `D` of the system is passed to the program as argument of the `-d` command-line option (such implementation is due to Prof. David Morse).

Single-phase SCF calculation requires two input files:

- a parameter file: `param`
- a command file: `command`

under the working directory, and their names have to be `param` and `command`, respectively.

When the program is executed, the parameter file is read first, which is used to initialize the state of the program and allocate memory. The command file is read and interpreted after the parameter file. The command file is in JSON format and contains a list of commands that are interpreted and executed in sequence, which controls the program flow after initialization. The contents and formats of these two types of file are explained in detail elsewhere (see **Parameter Files**, **Command Files**).

Calculation of the boundary between two phases

Here is an example of command-line usage of PSCF+ to calculate the boundry between two phases (where they have the same Helmholtz free-energy density) using the Ridders' method.

```
pg [-e] -d D1,D2
```

In the above, dimensionalities of the two phases, `D1` and `D2`, are passed to the program as arguments of the `-d` command-line option; use 0 for dimensionality of the disordered phase.

Two-phase SCF calculation requires three input files:

- two parameter files: `param1` and `param2`
- a command file: `command`

under the working directory, and their names have to be `param1`, `param2` (for the two phases having dimensionalities `D1` and `D2`, respectively) and `command`.