

How to Install MakePES

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NOTE

- MakePES is a command line based program. This manual assumes that you are familiar with the commands in UNIX, and that you are working on Bourne Shell (bash).
- “/path/to/sindo” indicates the absolute path of your installation directory. For example,

```
/path/to/sindo -> /home/yagi/pgm/sindo-4.0_220312
```

1. Install Java JDK in your system. For details, see “How to Install JSindo”.
2. Download `sindo-4.0_xxxx.zip` from our website
<https://tms.riken.jp/en/research/software/sindo>
3. Unzip (double click) the file, and find “`sindovars.sh`” in the top directory,

```
> cd sindo-4.0_xxxx
> ls
FSindo/   JSindo/   LICENSE   README.md  script/   sindovars.sh
```

Edit “`sindovars.sh`” and set “`/path/to/sindo`” to the name of install directory.

```
#!/bin/bash

export sindo_dir=/path/to/sindo
export CLASSPATH=${CLASSPATH}:${sindo_dir}/JSindo/jar/JSindo-4.0_fat.jar
export PATH=$PATH:${sindo_dir}/script:${sindo_dir}/FSindo/bin
export SINDO_RSH=ssh
```

4. Open a terminal, source “`sindovars.sh`”, and then invoke RunMakePES:

```
. /path/to/sindo/sindovars.sh
java RunMakePES -h
```

MakePES is successfully installed if you get the following message,

```
USAGE: java RunMakePES [ -f xmlfile ] [--input-version 1|2]
```

It is useful to source “sindovars.sh” in your ~/.bashrc,

4. Configuration for Gaussian

Note: You can skip this step if you don’t plan to use Gaussian, or if you run Gaussian by yourself.

Proceed to “script”, execute a configure script, and follow the instruction,

```
> cd sindo-4.0_xxxx/script  
> ./configure
```

You will be asked to enter a directory where Gaussian is installed, the version of Gaussian, and a local scratch directory. The script creates runGaussian.sh in the same directory.

Note that “sindovars.sh” sets a path to this directory:

```
export PATH=$PATH:$sindo_dir/script:$sindo_dir/FSindo/bin
```