

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).

Note:

MakePES is included in JSindo. So, you can go to step 5 if you have already set up JSindo.

1. Install Java in your system.

Visit Oracle Java (<https://www.java.com>) or Open JDK (<https://openjdk.java.net/>).

2. Download JAMA

Visit <https://math.nist.gov/javanumerics/jama/> and download Jama-1.0.3.jar

3. Download sindo-4.0.tar.gz from our website

<http://www.riken.jp/TMS2012/tms/en/research/software/sindo/index.html>

4. Extract the tar ball and go to sindo-4.0/jar,

```
> tar -zxvf sindo-4.0.tar.gz
> cd sindo-4.0/jar
> ls
JSindo-4.0.jar
```

Then, copy the jar file of JAMA.

```
> cp Jama-1.0.3.jar ./
```

5. Try the following command,

```
> export sindo_jar=/path/to/sindo-4.0/jar
> java -cp "$sindo_jar/*" RunMakePES -h
```

MakePES is successfully installed if you get the following message,

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

It is recommend to create an alias for a quick startup. Edit your ~/.bashrc and add the following two lines,

```
sindo_jar=/path/to/sindo-4.0/jar
alias RunMakePES='java -cp "$sindo_jar/*" RunMakePES'
```

After source, you can invoke the program by typing RunMakePES

```
> . ~/.bashrc
> RunMakePES -h
USAGE: java RunMakePES [ -f xmlfile ] [--input-version 1|2]
```

6. Configuration for Gaussian

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

Go to a folder "script", execute a configure script, and follow the instruction,

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

You will be asked to enter a folder where Gaussian is installed, the version of Gaussian, and a local scratch folder. The script creates runGaussian.sh in the same folder. Set a path to this folder so that MakePES can use runGaussian.sh.

```
> export PATH=${PATH}:/path/to/sindo-4.0/script
```

Again, it is recommended to add this line to ~/.bashrc.