How to Install JSindo

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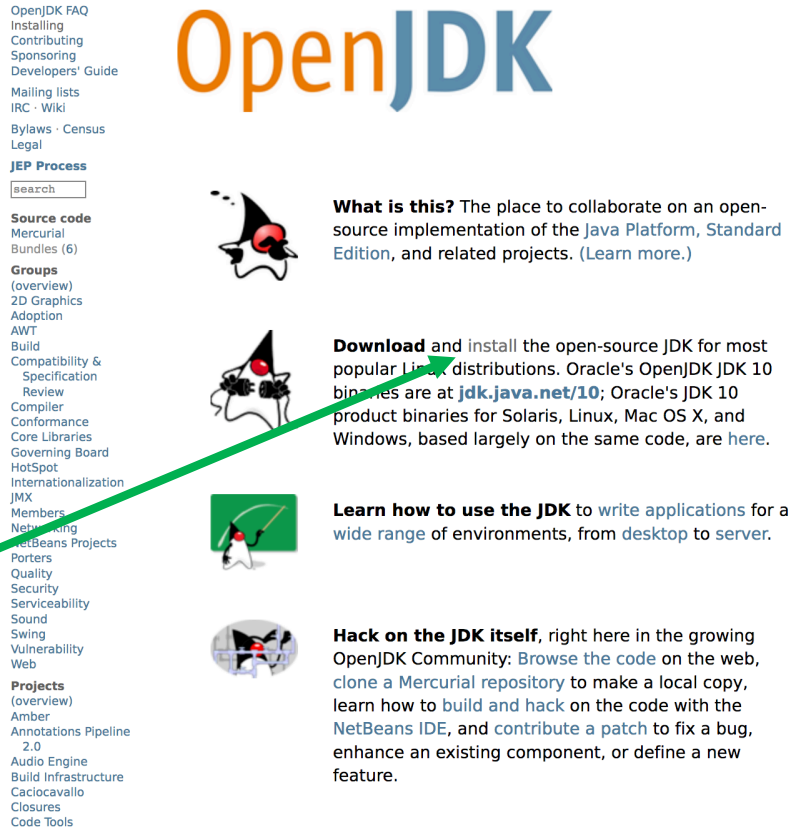
1. Install Java

Install Java of oracle (left), Open JDK (right), or any other.

https://www.java.com/en/

http://openjdk.java.net/

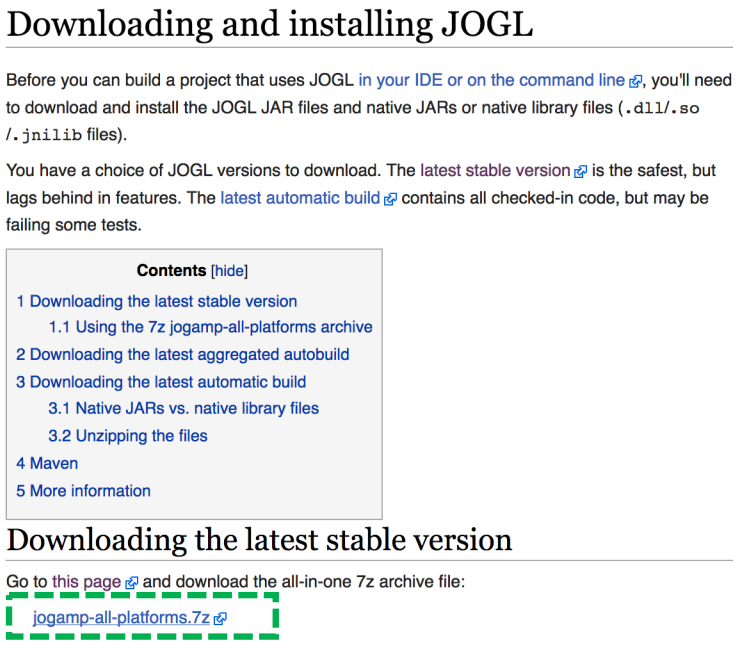


Click here and follow the instructions.

Note: Although Java 9 and 10 have been released since 2017/09 and 2018/03, respectively, Java 8 (1.8.x) is still recommended for JSindo, because it uses Java3D which may or may not be compatible with the newer Java.

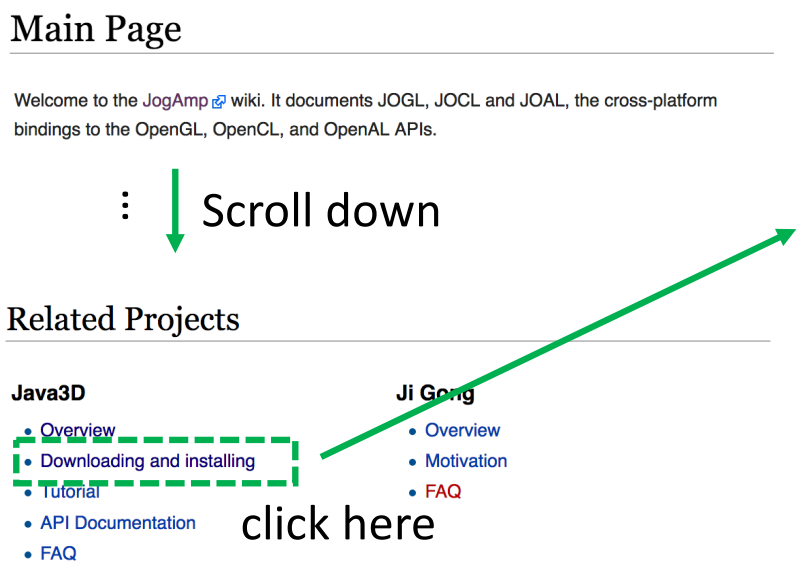
2. Setting up Java3D

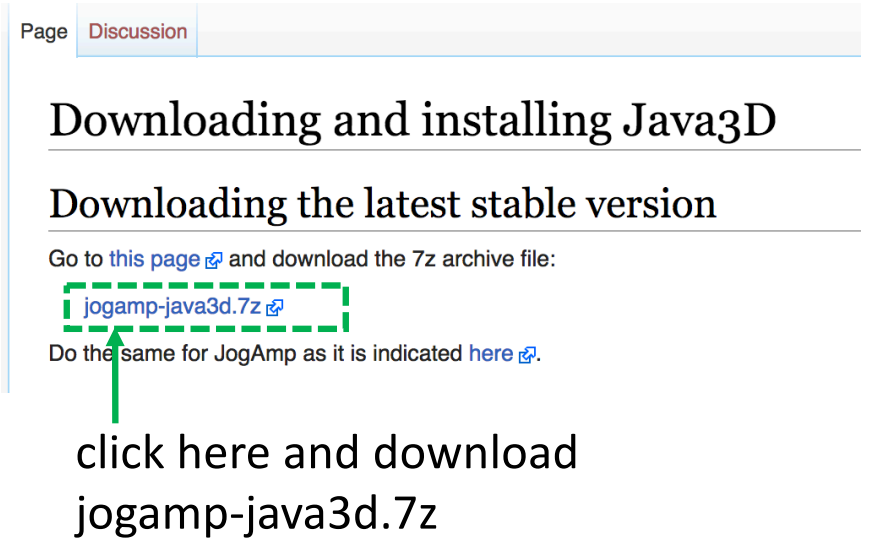
JSindo uses Java3D for visualization. A stable version, 1.6.0, is available from JogAmp. Goto http://jogamp.org



click here and download jogamp-all-platforms.7z

Go back to the Main page and scroll down





Unarchive the two files you've just downloaded. 7z files can be unarchived using, for example, "7Z Opener" (for Win) or "The Unarchiver" (for Mac), which are freely available.

7Z Opener
Tiny Opener

The Unarchiver
MacPaw Inc.

You will find jar files in jogamp-all-platforms/jar and in jogamp-java3d. The following jar files are needed for JSindo:

```
jogamp-all-platforms/jar/
     gluegen-rt.jar
     gluegen.jar
     gluegen-rt-natives-XXX.jar
     jogl-all.jar
     jogl-all-natives-XXX.jar
```

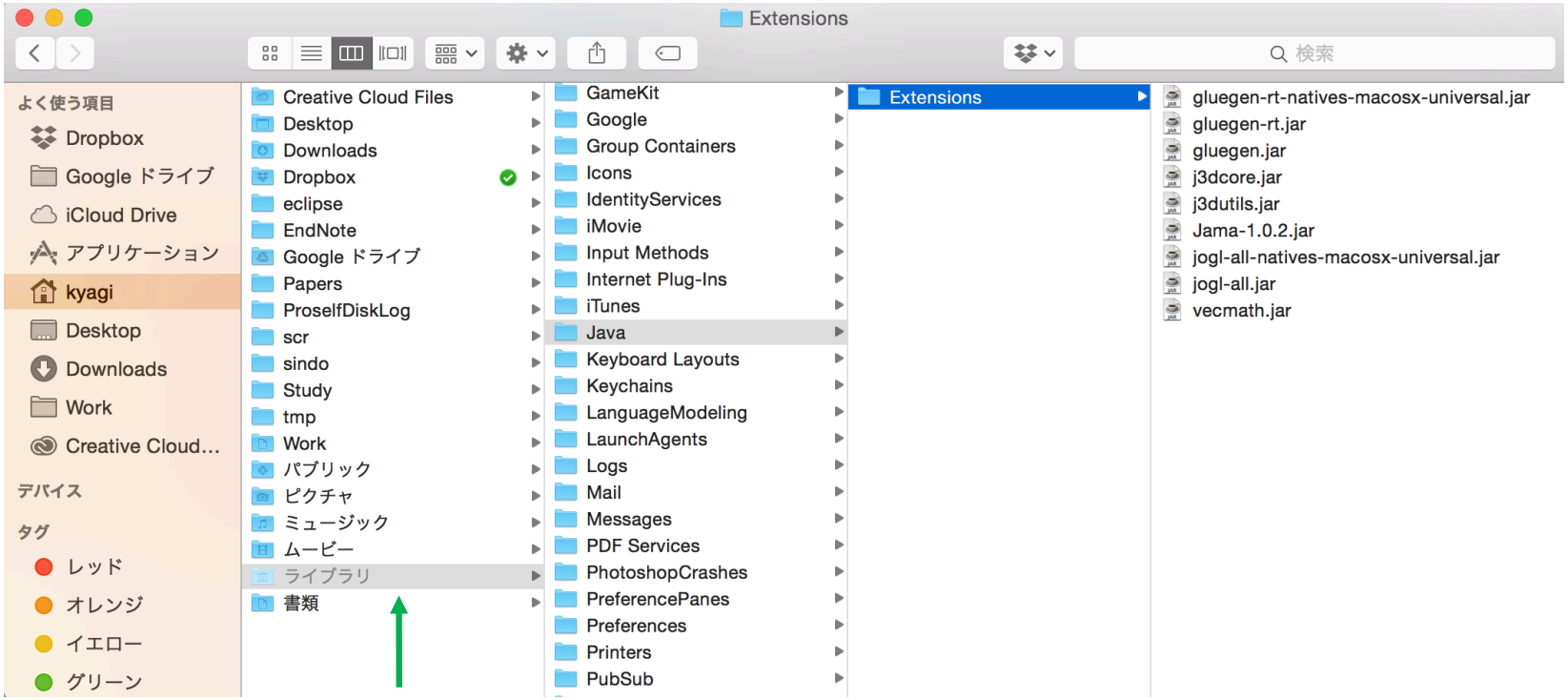
```
jogamp-java3d/
     j3dcore.jar
     j3dutils.jar
     vecmath.jar
```

where XXX indicates your OS and CPU.

We will next describe how to install these files in each platform.

MacOSX: XXX = macosx-universal.

The easiest install for MaxOSX is to copy the jar files to an extension folder. In MacOSX, it is set to ~/Library/Java/Extensions. Click Go menu of finder with opion key pressed (~/Library is hidden) and choose Library. Create the folder if you don‘t have it yet, then copy the jar files in this folder.



Windows: XXX = windows-amd64 or windows-i586

i586 is for 32-bit and amd64 is for 64-bit. Let's first check if your Java is 32- or 64-bit. In the DOS prompt, type "java -version" and you will see a message like this:

```
>java –version
java version "1.8.0_45"
Java(TM) SE Runtime Environment (build 1.8.0_45-b14)
Java HotSpot(TM) 64-Bit Server VM (build 25.45-b02, mixed mode)
```

This is an example of 64-bit. If "64-Bit" is absent, then it's 32-bit. (It doesn't explicitly state "32-Bit", unfortunately.)

Now, we will copy the jar files to an extension folder, which are located in

32-bit c:¥Program Files(x86)¥Java¥jre1.x.x_xxx¥lib¥ext
64-bit c:¥Program Files¥Java¥jre1.x.x_xxx¥lib¥ext

Copy the following jar files in this folder,

```
gluegen-rt.jar
gluegen.jar
gluegen-rt-natives-windows-xxx.jar
jogl-all.jar
jogl-all-natives-windows-xxx.jar
```

```
j3dcore.jar
j3dutils.jar
vecmath.jar
```

LINUX: XXX = linux-amd64 or linux-i586

(* CPU = armv6 and armv6hf are for ARM cpus, which are used for phones.)

i586 is for 32-bit and amd64 is for 64-bit. Let's first check if your Java is 32- or 64-bit. In the terminal, type "java -version" and you will see a message like this:

```
>java –version
openjdk version "1.8.0_121"
OpenJDK Runtime Environment (build 1.8.0_121-b13)
OpenJDK 64-Bit Server VM (build 25.121-b13, mixed mode)
```

This is an example of 64-bit. If "64-Bit" is absent, then it's 32-bit.

Now, we add the jar files to an environment variable CLASSPATH. If you are in bash,

```
JOGAMP_JAR=${HOME}/lib/jogamp-all-platforms/jar
export CLASSPATH=${CLASSPATH}:${JOGAMP_JAR}/gluegen.jar
export CLASSPATH=${CLASSPATH}:${JOGAMP_JAR}/gluegen-rt.jar
export CLASSPATH=${CLASSPATH}:${JOGAMP_JAR}/jogl-all.jar
export CLASSPATH=${CLASSPATH}:${JOGAMP_JAR}/gluegen-rt-natives-linux-xxx.jar
export CLASSPATH=${CLASSPATH}:${JOGAMP_JAR}/jogl-all-natives-linux-xxx.jar

J3D_JAR=${HOME}/lib/jogamp-java3d
export CLASSPATH=${CLASSPATH}:${J3D_JAR}/j3dcore.jar
export CLASSPATH=${CLASSPATH}:${J3D_JAR}/j3dutils.jar
export CLASSPATH=${CLASSPATH}:${J3D_JAR}/vecmath.jar
```

where xxx = amd64 or i586 for 64-bit or 32-bit, respectively. It would be a good idea to add these lines in your .bashrc, so that they take effect upon login.

3. Download JAMA

JAMA is a linear algebra library for JAVA. We use it for matrix maltiplications, diagonalization, and so on. It can be downloaded from,

https://math.nist.gov/javanumerics/jama/

Then, copy the jarfile to the extension folder or add to CLASSPATH as before.

4. Test JSindo

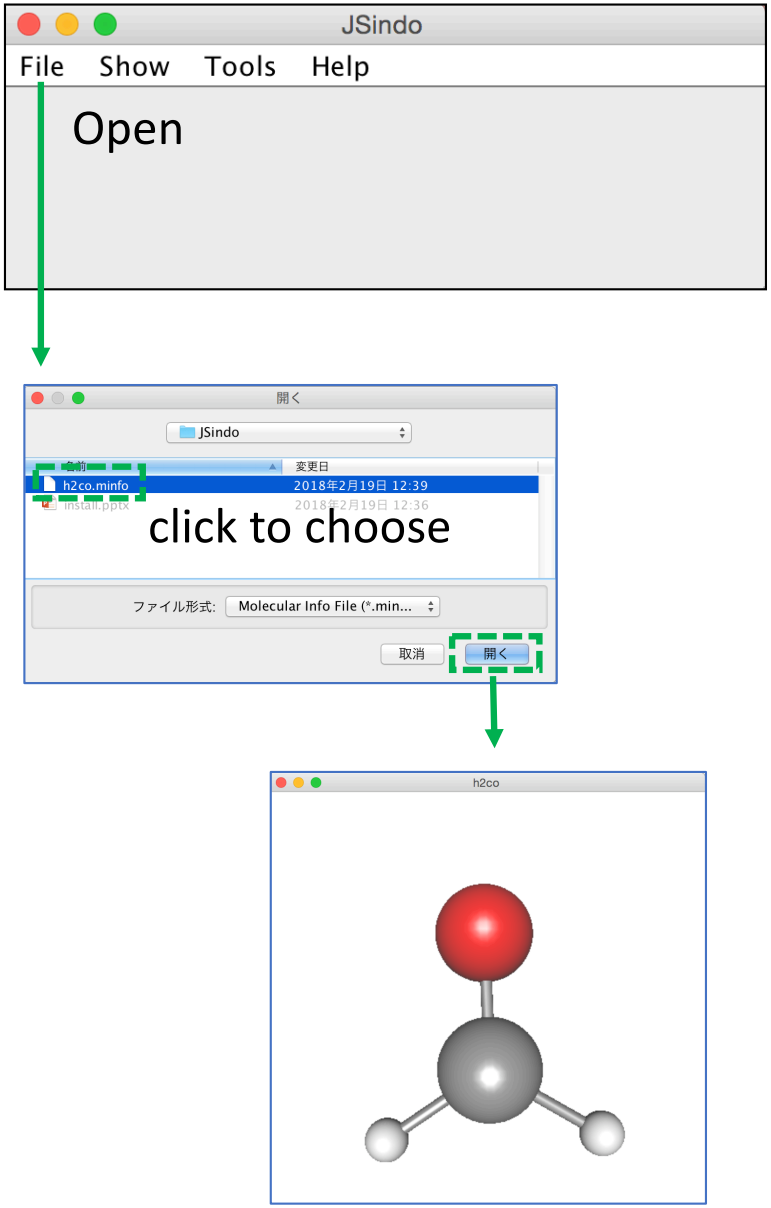
Now, double click JSindo-4.0_xxxxxx.jar. You should see a control panel of JSindo.

If you don't see the panel, review the installation of Java.

Let's open "sample/h2co.minfo", which comes with this document. It contains data of formaldehyde.

Click, File -> Open, choose "h2co.minfo", and click Open. If you see formaldehyde, you're done with the first step!

If this step fails, it is highly likely that Java3D has a problem. Double check if the jarfiles are set correctly, that is, copied to the extension folder or set to CLASSPATH.



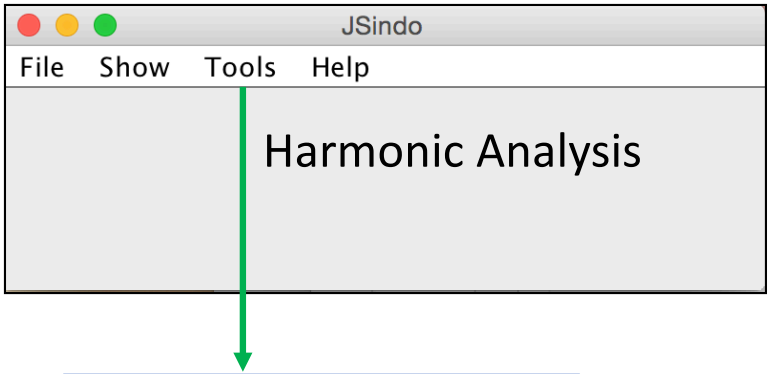
Finally, goto Tools -> Harmonic Analysis. This should create a panel of “Normal modes”.

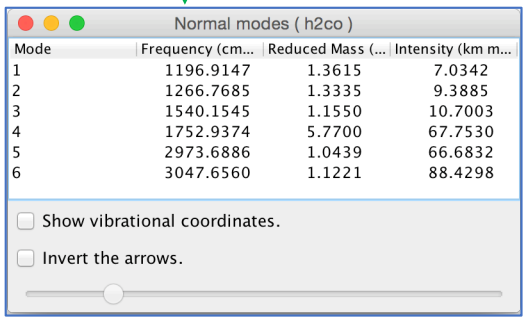
If you don’t see this panel, JAMA isn’t working. Check if the jarfile of JAMA is set correctly.

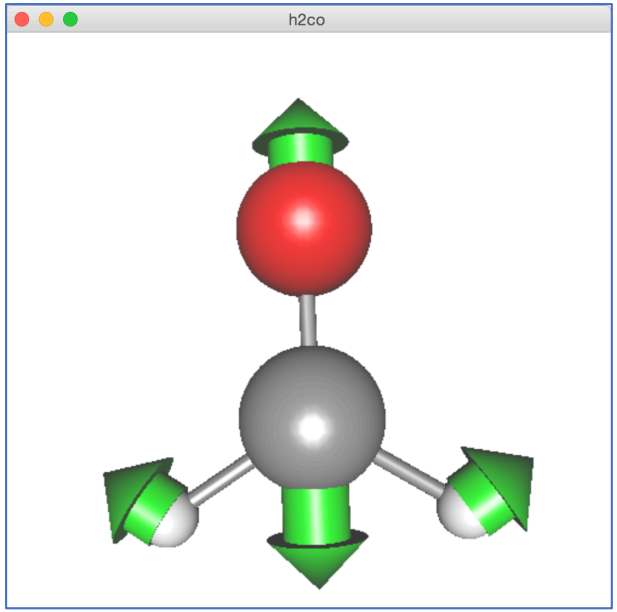
If the panel appears, you’re all set! Congradulations!

Check on ”show vibrational coordinates”, and choose a mode you want to see. Vibrational motion will be indicated by arrows. You can “Invert the arrows” by a check box, and change the magnitude using a slider.

Thanks for using JSindo!
Enjoy!







FAQ

1. I want to use JSindo from a command line.

   Use the following command:

```
>java –cp /path/to/JSindo-4.0_xxxxxx.jar JSindo
```

2. I cannot or don't want to copy jarfiles into an extension folder.

   Specify all jarfiles using ":" as a separator,

```
>java –cp JSindo-4.0_xxxxxx.jar:Jama-1.0.3.jar:... JSindo
```

3. Is there an alternative to "-cp"? The command is too long.

   The environment variable, CLASSPATH, does the same thing. Set CLASSPATH for all jarfiles,

```
> export CLASSPATH=${CLASSPATH}:/path/to/JSindo-4.0_xxxxxx.jar
> export CLASSPATH=${CLASSPATH}:/path/to/Jama-1.0.3.jar
...
```

   Then, you can start simply by,

```
> java JSindo
```

   I save the setting to ~/.bashrc, so that the CLASSPATH is configured upon login.