

How to Install JSindo for LINUX

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1. Install Java

Let's check if you have Java installed or not, and the version of Java if you have. 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)
```

If your Java is 1.8.xxx (=JDK8), then you can skip the installation and go to Chap. 2.

If your Java is a newer one, 1.9.xxx (=JDK9) and later, it is unfortunately **NOT** compatible with Java3D library, which JSindo use for visualization. You may either uninstall or switch to JDK8 keeping the current ones. Ask google for details.

To install JDK8, type in the terminal,

```
> yum install java-1.8.0-openjdk
```

(Fedora)

```
> apt-get install openjdk-8-jre
```

(Debian, Ubuntu)

See the OpenJDK website for further details.



What is this? The place to collaborate on an open-source implementation of the Java Platform, Standard Edition, and related projects. (Learn more.)



Download and install the open-source JDK for most popular Linux distributions. Oracle's OpenJDK JDK 10 binaries are at jdk.java.net/10/; Oracle's JDK 10 product binaries for Solaris, Linux, Mac OS X, and Windows, based largely on the same code, are here.



Learn how to use the JDK to write applications for a wide range of environments, from desktop to server.



Hack on the JDK itself, right here in the growing OpenJDK Community: Browse the code on the web, clone a Mercurial repository to make a local copy, learn how to build and hack on the code with the NetBeans IDE, and contribute a patch to fix a bug, enhance an existing component, or define a new feature.

<http://openjdk.java.net/>

Alternately, you may use Oracle Java 1.8.x. It is available from here.

Search “Java SE download” in Google and goto the following website.

<http://www.oracle.com/technetwork/java/javase/downloads/index.html>

ORACLE Menu

Oracle Technology Network / Java / Java SE / Downloads

Java SE Downloads

Java Platform, Standard Edition

Java SE 10.0.1

Java SE 10.0.1 is the latest feature release for the Java SE Platform

Installation Instructions

Release Notes

Oracle License

Java SE Licensing Information User Manual

Certified System Configurations

Readme

Which Java package

Software Developers: JDK (Java SE Development Kit). For Java Developers. Includes a complete JRE plus tools for developing, debugging, and monitoring Java applications.

Administrators: **Running applications on a server: Server JRE** (Server Java Runtime Environment) for deploying Java applications on servers. Includes tools for JVM monitoring and tools commonly required for server applications, but does not include browser integration (the Java plug-in), auto-update, nor an installer. [Learn more](#)

End user running Java on a desktop: **JRE**: (Java Runtime Environment). Covers most end-users needs. Contains everything required to run Java applications on your system.

Java SE 8u171/ 8u172

Java SE 8u171 includes important bug fixes. Oracle strongly recommends that all Java SE 8 users upgrade to this release. Java SE 8u172 is a patch-set update, including all of 8u171 plus additional bug fixes (described in the release notes). [Learn more](#)

JDK DOWNLOAD +

Server JRE DOWNLOAD +

JRE DOWNLOAD +

accept

Java SE Development Kit 8u172

You must accept the [Oracle Binary Code License Agreement for Java SE](#) to download this software.

Accept License Agreement Decline License Agreement

Product / File Description	File Size	Download
Linux ARM 32 Hard Float ABI	77.99 MB	jdk-8u172-linux-arm32-vfp-hflt.tar.gz
Linux ARM 64 Hard Float ABI	74.9 MB	jdk-8u172-linux-arm64-vfp-hflt.tar.gz
Linux x86	170.07 MB	jdk-8u172-linux-i586.rpm
Linux x86	184.91 MB	jdk-8u172-linux-i586.tar.gz
Linux x64	167.15 MB	jdk-8u172-linux-x64.rpm
Linux x64	182.08 MB	jdk-8u172-linux-x64.tar.gz
Mac OS X x64	247.87 MB	jdk-8u172-macosx-x64.dmg
Solaris SPARC 64-bit (SVR4 package)	140.05 MB	jdk-8u172-solaris-sparcv9.tar.Z
Solaris SPARC 64-bit	99.35 MB	jdk-8u172-solaris-sparcv9.tar.gz
Solaris x64 (SVR4 package)	140.63 MB	jdk-8u172-solaris-x64.tar.Z
Solaris x64	97.06 MB	jdk-8u172-solaris-x64.tar.gz
Windows x86	199.11 MB	jdk-8u172-windows-i586.exe
Windows x64	207.3 MB	jdk-8u172-windows-x64.exe

i586 and x64 is 32- and 64-bit, respectively. I think you will normally choose 64-bit.

2. Download Java3D

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

The screenshot shows the JogAmp website homepage. The navigation bar includes links for Home, Gluegen, JOAL, JOGL, JOCL, Wiki, Blogs, Streams, and Forum. The 'Wiki' link is highlighted with a green dashed box. A green arrow points from the 'Wiki' link to the 'Index of /deployment/jogamp-current/archive' page. Another green arrow points from the 'Builds / Downloads' section to the 'jogamp-all-platforms.7z' file in the index.

Index of /deployment/jogamp-current/archive

Name	Last modified	Size	Description
Parent Directory		-	
API-Changes/	2015-10-10 05:56	-	
ChangeLogs/	2015-10-10 05:43	-	
Sources/	2015-10-10 05:45	-	
gluegen-javadoc.7z	2015-10-09 06:20	393K	
joal-demos.7z	2015-10-10 05:01	1.2M	
joal-javadoc.7z	2015-10-09 06:21	107K	
jocl-demos.7z	2015-10-10 05:02	553K	
jocl-javadoc.7z	2015-10-10 03:27	182K	
jogamp-all-platforms.7z	2015-10-10 05:03	53M	
jogamp-fat-all.7z	2015-10-10 05:02	31M	
jogl-demos.7z	2015-10-10 05:02	25M	
jogl-javadoc.7z	2015-10-10 03:25	2.1M	
test-results/	2015-10-10 05:03	-	

Apache/2.4.25 (Debian) Server at jogamp.org Port 443

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

Go back to the main page, then go to Wiki page,

Scroll down the Wiki page,

Main Page

Welcome to the JogAmp [wiki](#). It documents JOGL, JOCL and JOAL, the cross-platform bindings to the OpenGL, OpenCL, and OpenAL APIs.

⋮ ↓ Scroll down

Related Projects

Java3D

- [Overview](#)
- [Downloading and installing](#)
- [Tutorial](#)
- [API Documentation](#)
- [FAQ](#)

Ji Gong

- [Overview](#)
- [Motivation](#)
- [FAQ](#)

click here

Page [Discussion](#)

Downloading and installing Java3D

Downloading the latest stable version

Go to [this page](#) and download the 7z archive file:

[jogamp-java3d.7z](#)

Do the same for JogAmp as it is indicated [here](#).

click here and download
jogamp-java3d.7z

Unarchive the two files you've just downloaded. 7z files can be unarchived by,

```
> 7za x jogamp-all-platforms.7z  
> 7za x jogamp-java3d.7z
```

If you don't have the command, install p7zip package,

```
> yum install p7zip
```

(Fedora)

```
> apt-get install p7zip
```

(Debian and Ubuntu)

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-linux-XXX.jar  
  jogl-all.jar  
  jogl-all-natives-linux-XXX.jar
```

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

where **XXX** = amd64 or i586 for 64 or 32-bit, respectively. You can 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.

3. Download JAMA

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

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

JAMA : A Java Matrix Package

[\[Background \]](#) [\[The Package \]](#) [\[Request for Comments \]](#) [\[Authors \]](#) [\[Related Links & Libraries \]](#)

Background

JAMA is a basic linear algebra package for Java. It provides user-level classes for constructing and manipulating real, dense matrices. It is meant to provide sufficient functionality for routine problems, packaged in a way that is natural and understandable to non-experts. It is intended to serve as *the* standard matrix class for Java, and will be proposed as such to the [Java Grande Forum](#) and then to [Sun](#). A straightforward public-domain reference implementation has been developed by the [MathWorks](#) and [NIST](#) as a strawman for such a class. We are releasing this version in order to obtain public comment. There is no guarantee that future versions of JAMA will be compatible with this one.

⋮ ↓ Scroll down

The Package

Version 1.0.3 (November 9, 2012)

- [Documentation](#)
- [Example](#)
- Source [[Jama-1.0.3.zip](#)] [[Jama-1.0.3.tar.gz](#)]
- Jar file [[Jama-1.0.3.jar](#)]
- [ChangeLog](#)

→ click here and download a jarfile.

4. Download and test JSindo

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

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

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 all jar files in this folder,

```
> cp /path/to/jogamp-all-platforms/jar/gluegen.jar ./
> cp /path/to/jogamp-all-platforms/jar/gluegen-rt.jar ./
> cp /path/to/jogamp-all-platforms/jar/jogl-all.jar ./
> cp /path/to/jogamp-all-platforms/jar/gluegen-rt-natives-linux-xxx.jar ./
> cp /path/to/jogamp-all-platforms/jar/jogl-all-natives-linux-xxx.jar ./

> cp /path/to/jogamp-java3d/j3dutils.jar ./
> cp /path/to/jogamp-java3d/j3dcore.jar ./
> cp /path/to/jogamp-java3d/vecmath.jar ./

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

where **xxx** = amd64 or i586 for 64-bit or 32-bit, respectively.

Then, type the following command to invoke JSindo:

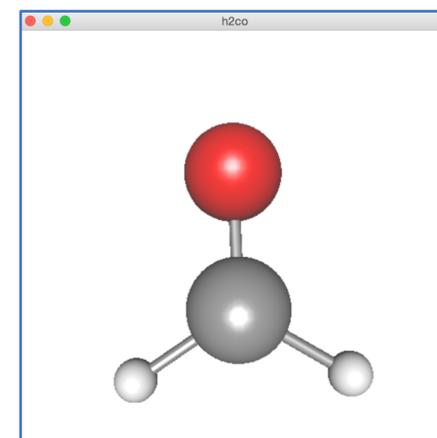
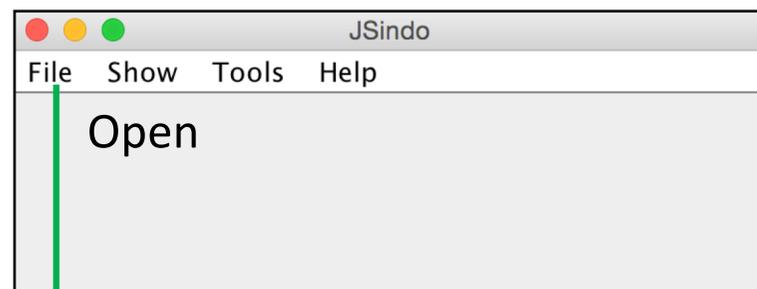
```
> export sindo_jar=/path/to/sindo-4.0/jar  
> java -cp "$sindo_jar/*" JSindo
```

With this command, you should see a control panel of JSindo. If you don't see the panel, review the installation of Java.

Let's test the program. Sample files are included in sindo-4.0/doc/sample_JSindo.

In JSindo control panel, 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 JogAmp/Java3D has a problem. Double check if the right jarfiles (xxx = amd64 or i586) are located in the folder.



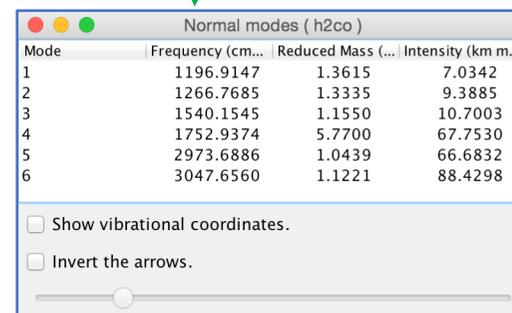
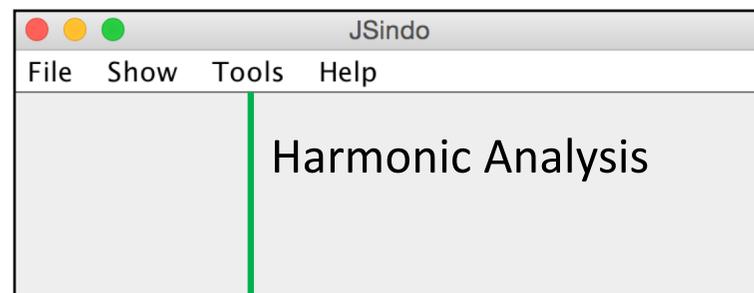
Finally, goto Tools -> Harmonic Analysis. This should create a panel of “Normal modes”.

If you don't see this panel, JAMA isn't working. Check if the jarfile of JAMA is located in the folder.

If the panel appears, you're all set! Congratulations!

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!



Mode	Frequency (cm...)	Reduced Mass (...)	Intensity (km m...
1	1196.9147	1.3615	7.0342
2	1266.7685	1.3335	9.3885
3	1540.1545	1.1550	10.7003
4	1752.9374	5.7700	67.7530
5	2973.6886	1.0439	66.6832
6	3047.6560	1.1221	88.4298

Show vibrational coordinates.
 Invert the arrows.

Slider: []

