# How to Install JSindo

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Theoretical Molecular Science Laboratory RIKEN Pioneering Research Cluster

2018/04/19

# Windows

# 1. Install Java

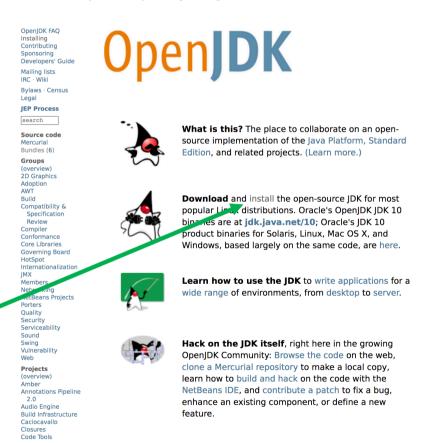
Install Java of Oracle (left), Open JDK (right), or any other.

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



Click here and follow the instructions.

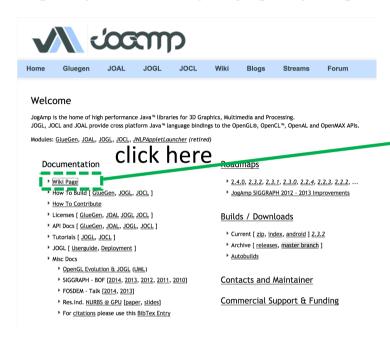
http://openjdk.java.net/



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. Download 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

#### Main Page

Welcome to the JogAmp & wiki. It documents JOGL, JOCL and JOAL, the cross-platform bindings to the OpenGL, OpenCL, and OpenAL APIs.

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#### Getting Started Community

- Downloading and installing
   Versioning and Releases
- Setting up a JogAmp project in your favorite IDE
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- Contribute to JogAmp
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#### Downloading and installing JOGL

Before you can build a project that uses JOGL in your IDE or on the command line &, you'll need to download and install the JOGL JAR files and native JARs or native library files (.dll/.so /.inilib files).

You have a choice of JOGL versions to download. The latest stable version  $\underline{\mathscr{C}}$  is the safest, but lags behind in features. The latest automatic build  $\underline{\mathscr{C}}$  contains all checked-in code, but may be failing some tests.

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  - 1.1 Using the 7z jogamp-all-platforms archive
- 2 Downloading the latest aggregated autobuild
- 3 Downloading the latest automatic build
  - 3.1 Native JARs vs. native library files
- 3.2 Unzipping the files
- 4 Maven
- 5 More information

#### Downloading the latest stable version

Go to this page of and download the all-in-one 7z archive file:

jogamp-all-platforms.7z &

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Unarchive the two files you've just downloaded. 7z files can be unarchived using, for example, "7Z Opener"



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

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

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

# 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/

### 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 <u>Java Grande Forum</u> and then to <u>Sun</u>. A straightforward public-domain reference implementation has been developed by the <u>MathWorks</u> and <u>NIST</u> 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.

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#### 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 [ <u>Jama-1.0.3.jar</u> ]
- ChangeLog

click here and download a jarfile.

# 4. Install jar files

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:\frac{\text{2.5} c:\text{2.5} c:\te
```

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
Jama-1.0.3.jar
```

where XXX = amd64 (64-bit) or i586 (32-bit).

### 5. Test JSindo

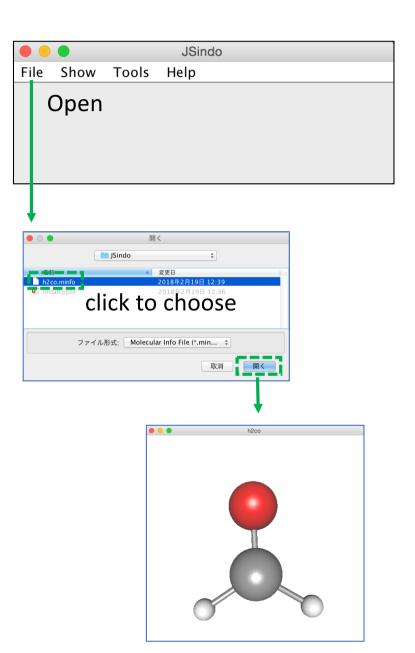
Now, double click JSindo-4.0.jar. You should see a control panel of JSindo.

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!

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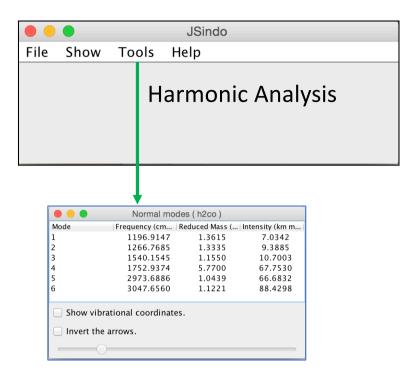
Finally, goto Tools -> Harmonic Analysis. This should create a panel of "Normal modes".

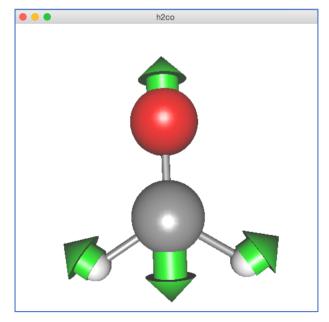
If you don't see this panel, JAMA isn't working. Make sure the jarfile of JAMA is copied to the right extension folder.

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!





# Mac

### 1. Install Java

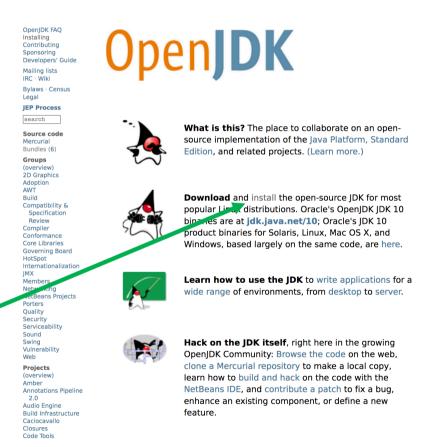
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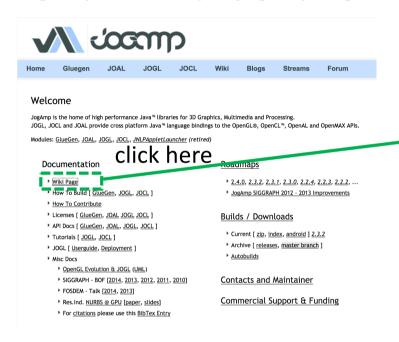
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Note: Although Java 9 and 10 have been released since 2017/09 and 2018/03, respectively, Java 8 (1.8.x) is still recommended for JSindo, because it uses Java3D which may or may not be compatible with the newer Java.

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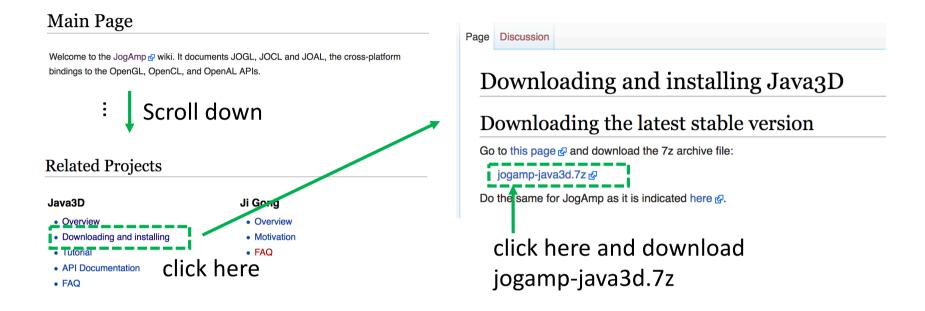
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```

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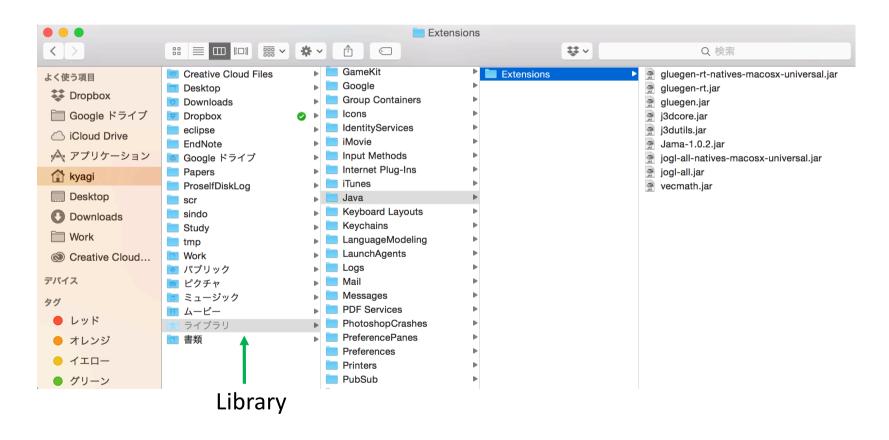
Version 1.0.3 (November 9, 2012)

- Documentation
- Example
- Source [ <u>Jama-1.0.3.zip</u> ] [ <u>Jama-1.0.3.tar.gz</u> ]
- Jar file Jama-1.0.3.jar ]
- ChangeLog

click here and download a jarfile.

# 4. Install jar files

The easiest way of install is to copy the jar files to an extension folder, which is set to ~/Library/Java/Extensions. Click Go menu of finder with <u>opion key pressed</u> (~/Library is hidden) and choose Library. Create the folder if you don't have it yet, then copy the jar files in this folder.



### 5. Test JSindo

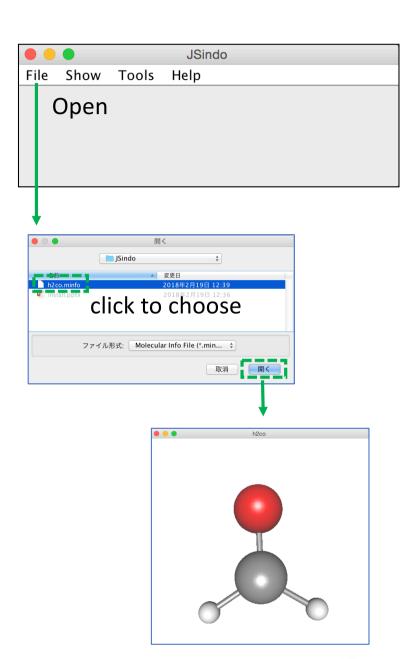
Now, double click JSindo-4.0.jar. You should see a control panel of JSindo.

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

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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 copied to the right extension folder or set to CLASSPATH.



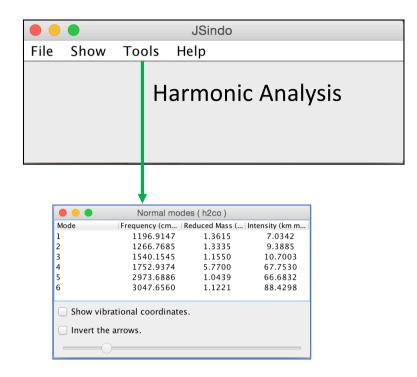
Finally, goto Tools -> Harmonic Analysis. This should create a panel of "Normal modes".

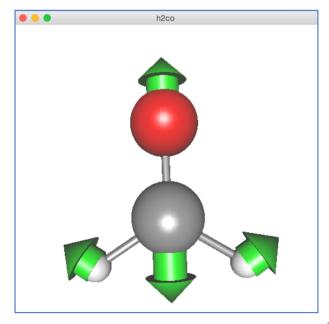
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Thanks for using JSindo! Enjoy!





# Linux

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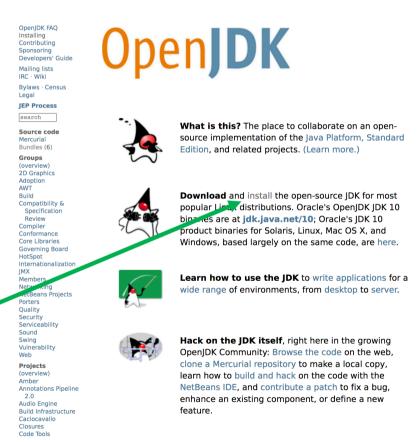
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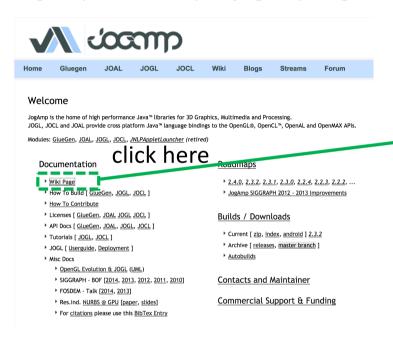
http://openjdk.java.net/



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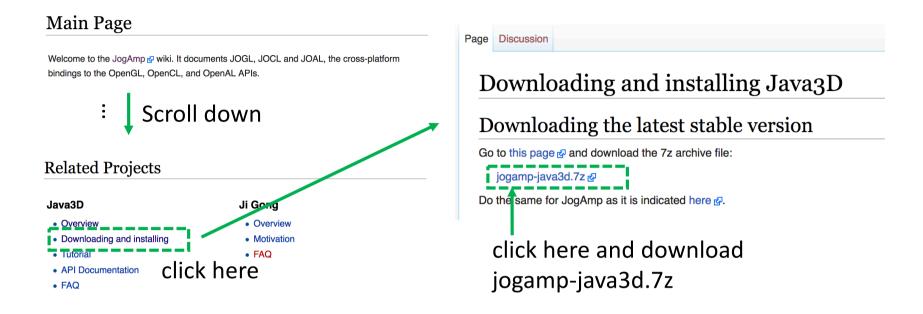
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```
> 7za e jogamp-all-platforms.7z
> 7za e jogamp-java3d.7z
```

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

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    gluegen.jar
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```

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

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

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

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- Jar file [ <u>Jama-1.0.3.jar</u> ]
- ChangeLog

click here and download a jarfile.

# 4. Setup the jar files

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

export CLASSPATH=${CLASSPATH}:${HOME}/lib/jama/Jama-1.0.3.jar
```

where xxx = amd64 or i586 for 64-bit or 32-bit, respectively. You may want to add these lines in your  $^{\sim}$ /.bashrc, so that they take effect upon login.

### 5. Test JSindo

Use the following command:

1. 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_xxxxxxx.jar:Jama-1.0.3.jar:... JSindo
```

2. 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,
```

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

# 5. Test JSindo

Type the following command to invoke JSindo:

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

Alternately, you may add in your ~/.bashrc as before,

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

Then, you can simply start by,

```
> java JSindo
```

With this command, you should see a control panel of JSindo.

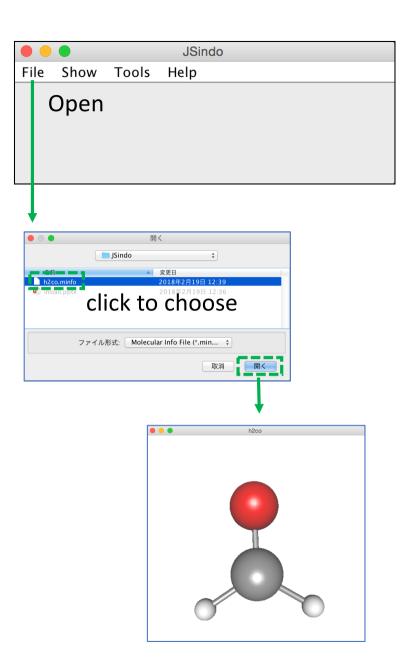
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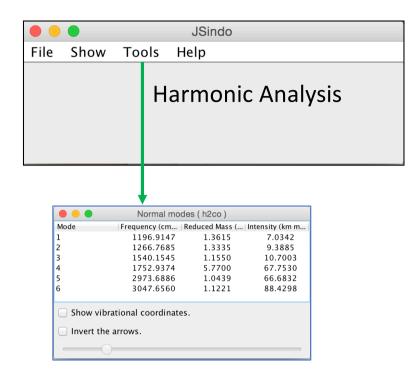
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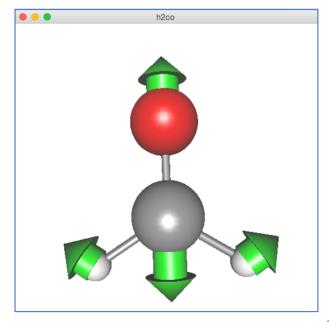
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# FAQ

#### 1. Fonts and Icons are too tiny.

Although we are aware of this problem that most likely happens in Win 10 (and perhaps Linux) with a high DPI diplay, we don't know the solution at this moment. This seems to be a general issue of Java/Swing applications, which some people says it is fixed in JRE9. However, JRE9 is reported to be incompatible with JogAmp/Java3D.

Your feedback on this issue is greatly appreciated!