

Installation Guide

Downloading JGromacs

The entire JGromacs package can be downloaded from our website as a single JAR (Java ARchive) file; *jgromacs_v1_bin.jar*. This file contains all binaries of the library.

(Note that the source code of the package can also be downloaded in the gzipped tar file; *jgromacs_v1_src.tgz*.)

In order to make use of the API in your own Java project or to run the example codes or the JUnit test suite available on our website, you will need to add the *jgromacs_v1_bin.jar* file to the classpath you are using.

First of all, download the jar file and place it in a directory where you can access it later. Here we give instructions for how to use the API in your project, compile and run example codes and the test suite.

Important:

The following instructions are valid only if you are compiling/running your code in Linux or Mac OS X. In case you are working in Windows, you will need to replace colon (:) characters with semicolon (;) characters in the commands below!

Using the API

In order to use the API in your own Java project, you only have to add the *jgromacs_v1_bin.jar* file as an external library to the build path of your project. In the commonly used development environments (IDEs) such as Eclipse, this can easily be done using a GUI.

Alternatively, you may compile your application in the command line using the following command:

```
javac -cp XXX/jgromacs_v1_bin.jar:. MainClass.java
```

Here **XXX** represents the path of location where the *jgromacs_v1_bin.jar* package has been downloaded to. **MainClass.java** is the class to be compiled.

Once compiled, your application can be run using the command:

```
java -cp XXX/jgromacs_v1_bin.jar:. MainClass
```

Alternatively, you can compile and run your application by rebuilding the JGromacs source code library using the following command:

```
javac -source 1.5 -cp YYY: MainClass.java
```

```
java -cp YYY: MainClass
```

Here **YYY** represents the path of location where the *jgromacs_v1_src.tgz* package has been extracted to.

Note that if you make use of JGromacs classes in your code, you need to import the required classes within your .java file. For example, the following command imports the `jgromacs.data.Structure` class into your source code:

```
import jgromacs.data.Structure;
```

Alternatively, you can import the entire `jgromacs.data` subpackage:

```
import jgromacs.data.*;
```

Compiling and running the example codes

The library of example codes can be downloaded as a gzipped tar file; *jgromacs_v1_examples.tgz*. This file also contains an example dataset used by the examples included in the package.

As a first step, unpack the `tgz` file:

```
tar xvzf jgromacs_v1_examples.tgz
```

This will give you the directory *examples/* containing 7 subdirectories.

Subdirectories *examples/data*, *examples/input*, *examples/output*, *examples/analysis*, *examples/advanced* and *examples/ui* contain example java files organized by topic.

In addition, the subdirectory *examples/dataset* contains the sample dataset required for running the example codes.

In order to compile and run an example code (for instance, `input/ReadStructures.java`), use the following commands in the *examples* directory:

```
javac -source 1.5 -cp XXX/jgromacs_v1_bin.jar: input/ReadStructures.java
```

```
java -cp XXX/jgromacs_v1_bin.jar: input/ReadStructures
```

Here **XXX** represents the path of location where the *jgromacs_v1_bin.jar* package has been downloaded to.

(Note that compiling example codes may give a list of warnings about variables that are never read. These warnings can be ignored as these codes are not complete programs but only illustrations of the exact usage of JGromacs methods.)

Running the JUnit Test Suite

A comprehensive JUnit Test Suite can be downloaded as a gzipped tar file; *kgromacs_v1_test.tgz*. The suite contains 21 test classes with 342 test methods.

As a first step, extract the gzipped tar file:

```
tar xvzf kgromacs_v1_test.tgz
```

This will give you the directory *test/* which contains binaries (.class files), source codes (.java files) and an example dataset (in the subdirectory *test\dataset*) required for running the test suite.

To run the tests with the `junit.textui.TestRunner` tool, use the following command in the directory *test/*:

```
java -cp XXX/kgromacs_v1_bin.jar:junit-4.10.jar:. junit.textui.TestRunner AllTests
```

Here `XXX` represents the path of location where *kgromacs_v1_bin.jar* has been downloaded to. (There should be a space after the period and before “`junit.textui...`”.)

Note that 2 of the 342 test methods depend on Gromacs installation as they have been designed to test those methods of the package that are dependent on Gromacs. This means that two tests will fail unless you set up your Gromacs environment. The remaining 340 test methods can be executed independently of Gromacs.