

Version
1.2

pbdR Core Team

Setting up a pbdR Environment

Installing MPI, R, and pbdR

Setting Up a pbdR Environment

Installing MPI, R, and pbdR

Version 1.2

Prepared by the pbdR Core Team:

Drew Schmidt

*Remote Data Analysis and Visualization Center,
University of Tennessee, Knoxville*

Wei-Chen Chen

*Department of Ecology and Evolutionary Biology,
University of Tennessee, Knoxville*

Pragneskumar Patel

*Remote Data Analysis and Visualization Center,
University of Tennessee, Knoxville*

George Ostrouchov

*Computer Science and Mathematics Division,
Oak Ridge National Laboratory*

© 2013-2014 pbdR Core Team. All rights reserved.

Permission is granted to make and distribute verbatim copies of this manual provided the copyright notice and this permission notice are preserved on all copies.

Permission is granted to copy and distribute modified versions of this manual under the conditions for verbatim copying, provided that the entire resulting derived work is distributed under the terms of a permission notice identical to this one.

Permission is granted to copy and distribute translations of this manual into another language, under the above conditions for modified versions, except that this permission notice may be stated in a translation approved by the pbdR Core Team.

This publication was typeset using L^AT_EX.

Contents

1	Allocation	1
2	Quick Introduction	1
2.1	Installing R	1
2.2	Installing MPI	1
2.3	Installing pbdR Packages	1
3	Mac OS X	2
3.1	Installing R	2
3.1.1	Installing from a Binary Package	2
3.1.2	Compiling from Source	7
3.2	Installing MPI	7
3.2.1	Installing from a MacPorts	8
3.2.2	Compiling from Source	8
3.3	Installing pbdR Packages	8
3.3.1	Installing from CRAN	8
3.3.2	Installing from the Shell	8
3.3.3	Installing from Github	8
4	Running pbdR Scripts	9
5	Installation Problems	10
5.1	R and MPI	10
5.2	pbdR	10

1 Allocation

We have tried to make the installation process as simple as possible, and these instructions as thorough as possible. However, this is not an entirely labor-free procedure, and does not even get into the really difficult side of large-scale computing: managing the system.

If you affiliated with a United States institution and are engaged in research that requires large-scale computing resources, [we encourage you to consider getting an allocation with us](#) . Not only can we tailor our pbdR development to help your research, but we can manage the hardware, operating system, and software utilities for you, so that you can focus entirely on the thing that matters, your research.

2 Quick Introduction

In this guide, we will detail the necessary steps for how to set up a pbdR environment. What follows in the remaining sections is a very lengthy list of installation instructions; however, most users should find the process fairly straight-forward, and may not need (or want) all of the details we will provide unless something goes wrong. In any case, the short version for setting up a pbdR environment is to:

1. install R ; see <http://cran.r-project.org/>
2. install an MPI library; <http://www.open-mpi.org/>, or <http://www.mpich.org/> for Windows
3. install the pbdR packages; see <http://r-pbd.org/>

Items 1 and 2 are interchangeable, and so if you already have R and/or an MPI library installed, then merely skip this/these step(s); there is no need to reinstall anything.

2.1 Installing R

This should be fairly painless. R has binary packages for every operating system you have heard of (and some you haven't), and the install should go fine. Of course, since R is open source, you are free to compile it yourself, should have have reason or need to do so. You can find both the source as well as binaries at the R project's main site: <http://cran.r-project.org/>.

Additionally, you may wish to customize your R build by compiling from source. For example, you may wish to link R with a high performance linear algebra library, such as MKL. See the *R Installation and Administration Manual* at <http://cran.r-project.org/doc/manuals/R-admin.html> for full details.

2.2 Installing MPI

For Linux and Mac users, we recommend installing OpenMPI, which is available from <http://www.open-mpi.org/> in both binary and source formats.

2.3 Installing pbdR Packages

All released pbdR packages are available from <http://cran.r-project.org/> which is the Comprehensive R Archive Network (CRAN). This is similar to the CPAN for perl or CTAN for L^AT_EX, although with many improvements and benefits over its competitors.

It is also possible to link pbdR with high performance linear algebra libraries, such as MKL. Figure 1 offers some insight into the package organization. See the pbdSLAP vignette for more details.

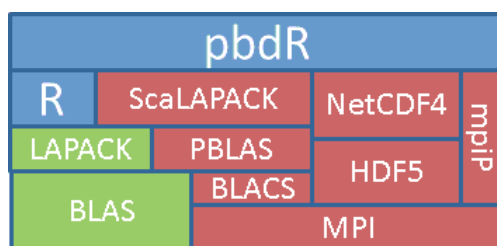


Figure 1: pbdR Relationships to Libraries

3 Mac OS X

Before starting, make sure you have installed Apple's [XCode](#) package. You can find this in the Mac App Store. Additionally, during the course of installation, you may need to use the terminal once or twice. You can launch it from Finder by navigating to the Applications folder; it should be called Terminal.app. If you have never used the terminal before, you might consider skimming [this simple guide](#) on terminal basics.

If you are completely new to R, then you might consider reading (or at least skimming) this useful guide, [R for Mac OS X FAQ](#). There is also the [R FAQ](#) which may also be useful for those who know very little about R. To learn more about programming with R, then you may find the [Introduction to R](#) guide useful.

3.1 Installing R

You can install R either from the binary package that CRAN builds (recommended) or from source.

3.1.1 Installing from a Binary Package

1. First you should download R from the official distribution site: <http://cran.r-project.org/bin/macosx/>

This directory contains binaries for a base distribution and packages to run on Mac OS X (release 10.6 and above). Mac OS 8.6 to 9.2 (and Mac OS X 10.1) are no longer supported but you can find the last supported release of R for these systems (which is R 1.7.1) [here](#). Releases for old Mac OS X systems (through Mac OS X 10.5) and PowerPC Macs can be found in the [old](#) directory.

Note: CRAN does not have Mac OS X systems and cannot check these binaries for viruses. Although we take precautions when assembling binaries, please use the normal precautions with downloaded executables.

R 3.0.0 "Masked Marvel" released on 2013/04/03

This binary distribution of R and the GUI supports 64-bit Intel based Macs on Mac OS X 10.6 (Leopard) or higher.

Since R 3.0.0 the binary is a single-arch build and contains only the x86_64 (64-bit Intel) architecture. PowerPC Macs and 32-bit Macs are only supported by building from sources or by older binary R versions. The default package type is "mac.binary" and the binary repository layout has changed accordingly.

Please check the MD5 checksum of the downloaded image to ensure that it has not been tampered with or corrupted during the mirroring process. For example type

```
md5 R-3.0.0.pkg
```

in the *Terminal* application to print the MD5 checksum for the R-3.0.0.pkg image. On Mac OS X 10.7 and later you can also validate the signature using `pkgutil --check-signature R-3.0.0.pkg`

Files:

[R-3.0.0.pkg](#) (latest version)
MD5-SHA256: 70d8a3b49d9b5c84d7050985416a (ca. 64MB)

[Mac-GUI-1.60.tar.gz](#)
MD5-SHA256: 09a16152d2d670720035616209a49

[NEWS](#) (for Mac GUI)

The new R.app Cocoa GUI has been written by Simon Urbanek and Stefano Iacus with contributions from many developers and translators world-wide, see "About R" in the GUI.

Subdirectories:

[tools](#)

[contrib](#)

[leopard](#)

[universal](#)

R 3.0.0 binary for Mac OS X 10.6 (Snow Leopard) and higher, signed package. Contains R 3.0.0 framework, R.app GUI 1.60 in 64-bit for Intel Macs. The above file is an installer package which can be installed by double-clicking. Depending on your browser, you may need to press the control key and click on this link to download the file.

This package contains the R framework, 64-bit GUI (R.app) and Tcl/Tk 8.6.0 X11 libraries. The latter component is optional and can be omitted when choosing "custom install", it is only needed if you want to use the `tkTK` R package. GNU Fortran is **NOT** included (needed if you want to compile packages from sources that contain FORTRAN code) please see [the tools directory](#).

Sources for the R.app GUI 1.60 for Mac OS X. This file is only needed if you want to join the development of the GUI, it is not intended for regular users. Read the INSTALL file for further instructions.

News features and changes in the R.app Mac GUI

Additional tools necessary for building R for Mac OS X:
Universal GNU Fortran compiler for Mac OS X (see [R for Mac tools page](#) for details).
Binaries of package builds for Mac OS X 10.6 or higher (Snow Leopard build)
Legacy binaries of universal (32-bit and 64-bit) package builds for Mac OS X 10.5 or higher (Leopard build)
Legacy binaries of universal (32-bit) package builds for Mac OS X 10.4 (Tiger build)

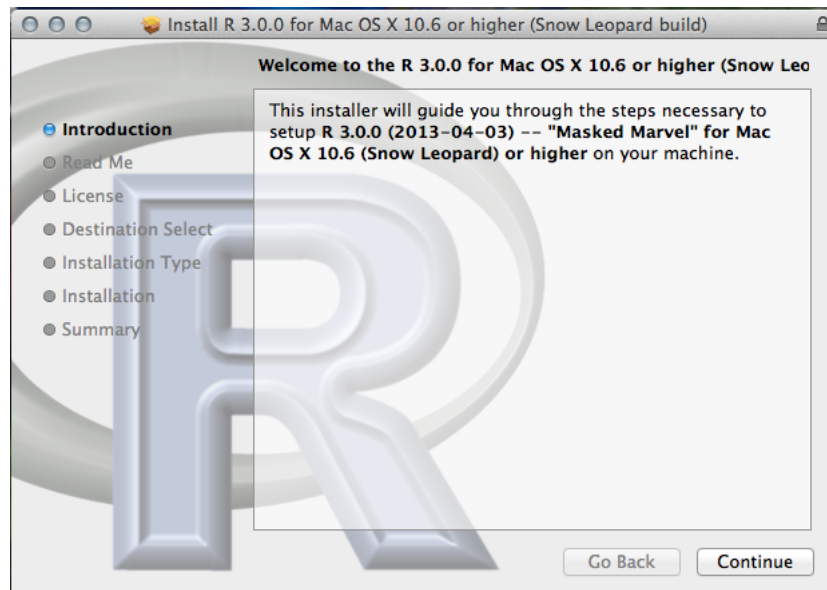
Download the R dmg package for Mac OS X. We recommend grabbing the latest version of R available.

[R-3.0.0.pkg](#) (latest version)
MD5-hash: 7c26aa38e940b6c84cf9f50098541fca
(ca. 64MB)

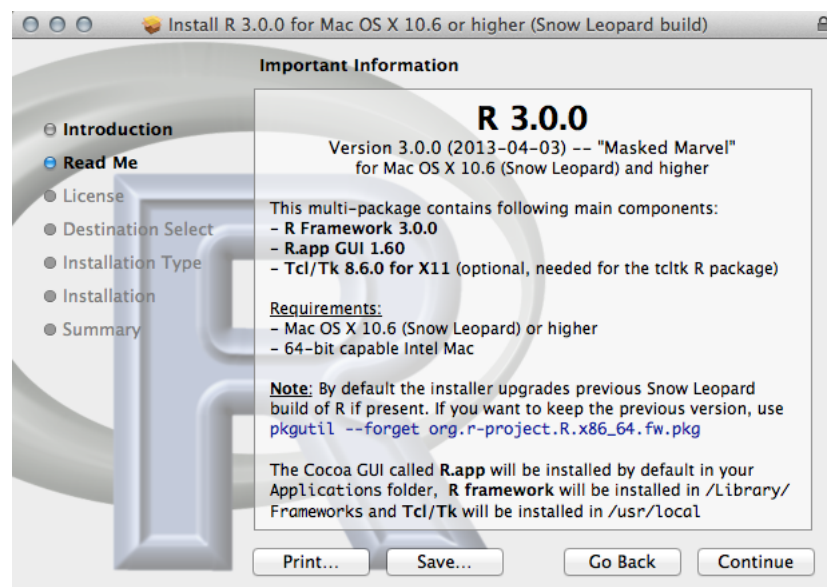
R 3.0.0 binary for Mac OS X 10.6 (Snow Leopard) and higher, signed package. C Intel Macs. The above file is an Installer package which can be installed by double press the control key and click on this link to download the file.

This package contains the R framework, 64-bit GUI (R.app) and Tcl/Tk 8.6.0 X11: omitted when choosing "custom install", it is only needed if you want to use the (needed if you want to compile packages from sources that contain FORTRAN cc

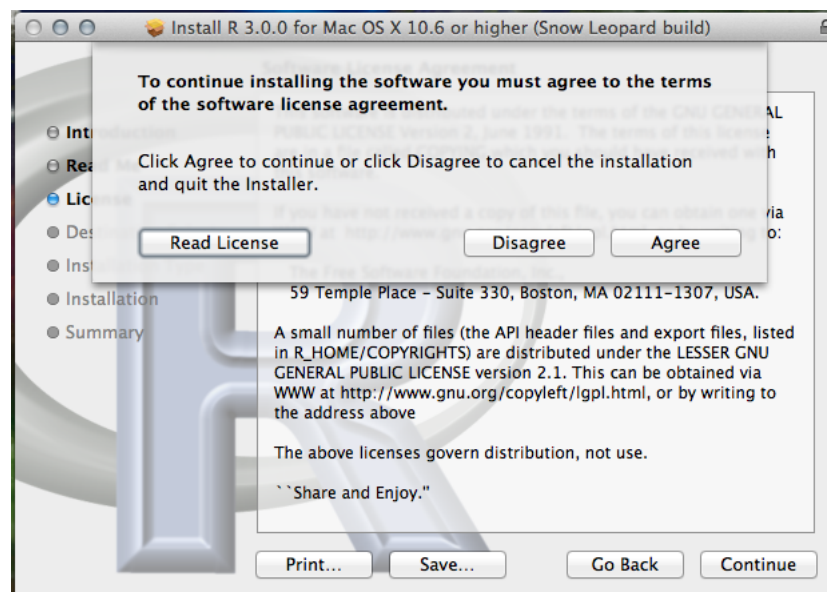
2. Open the saved file from 1 above to begin the installation. At the first setup screen, click 'Continue' to begin the installation process.



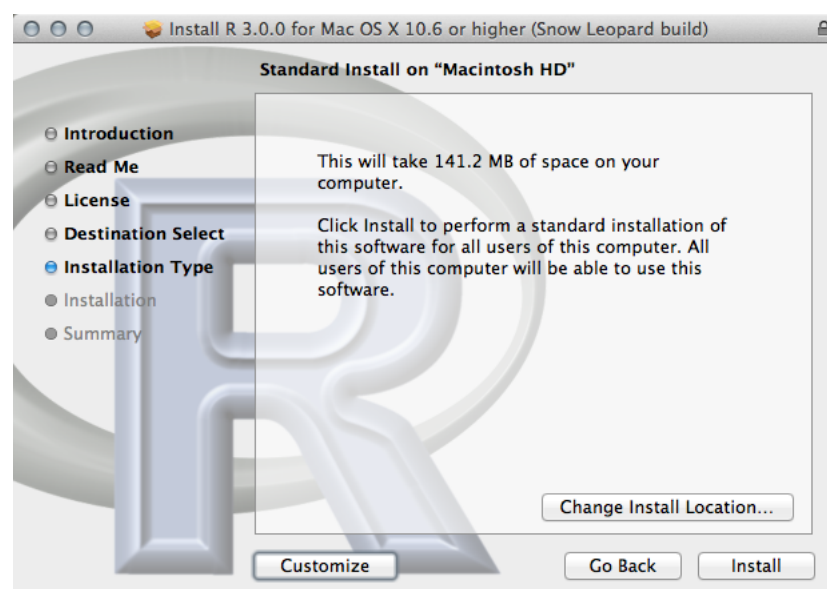
3. At the 'Read Me' section, read the important information and then click 'Continue'.



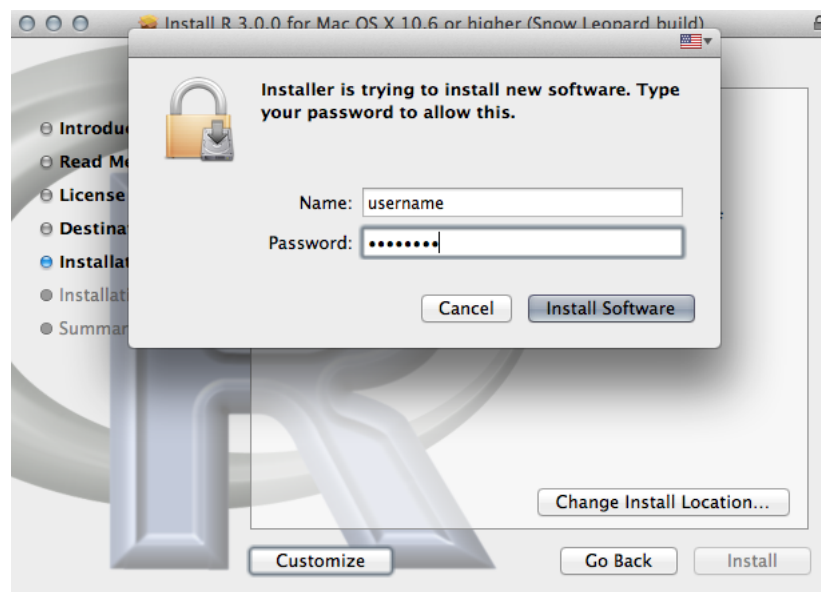
4. When prompted with the software license agreement, you must click 'Agree' to proceed. R is distributed under a free, "copyleft" license (GPL v3). You can read the license by clicking 'Read License'. Once you agree to the terms, click 'Agree'.



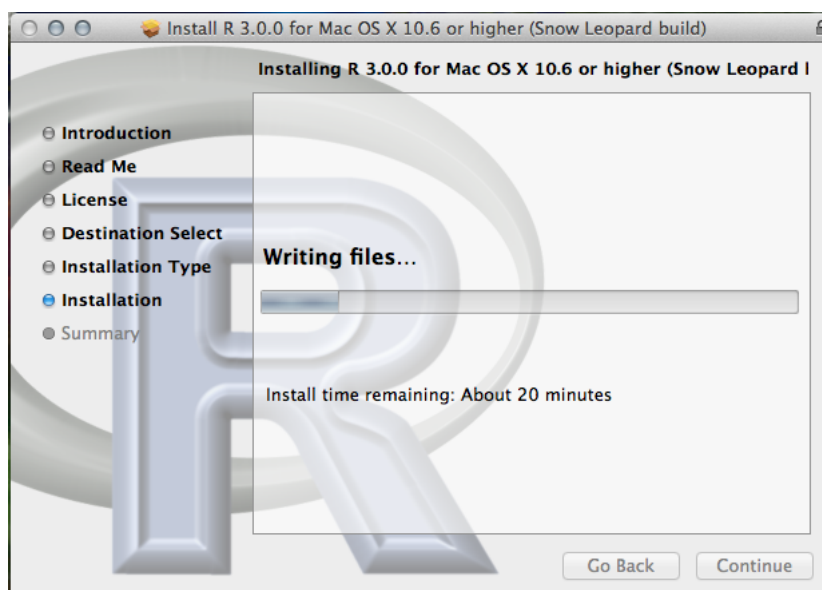
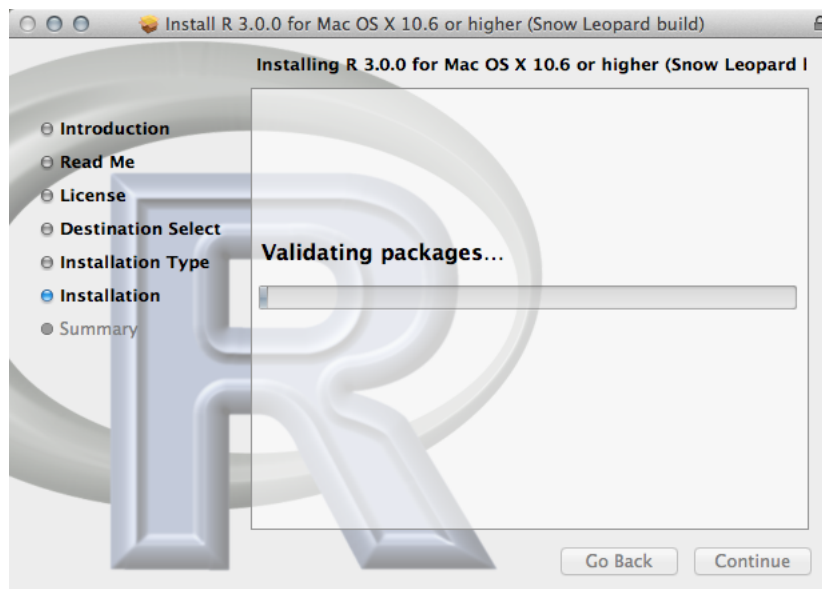
5. From the 'Installation Type' section, we recommend you use the defaults. However, you may change the install location by selecting 'Change Install Location...'. Once you have made your choice, click 'Install'.

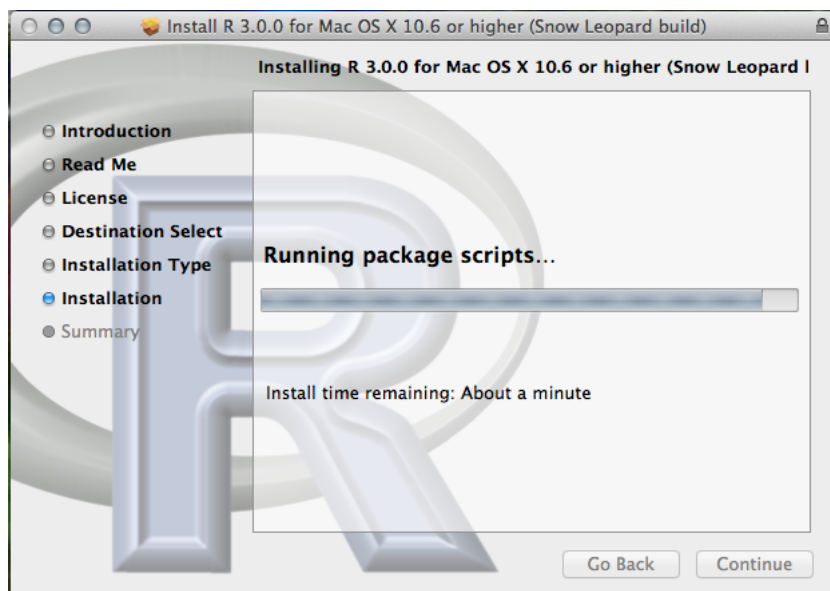
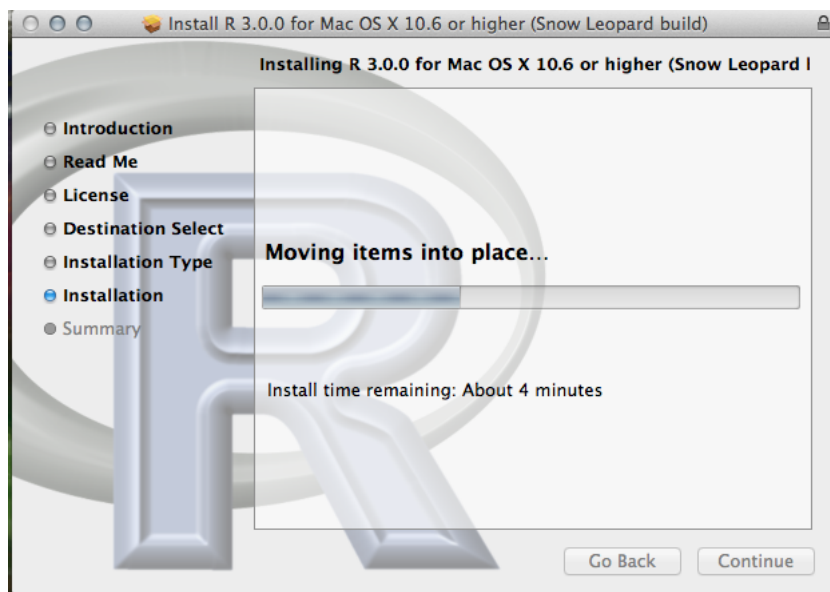


6. Next, you will be prompted for your computer's name and password. Enter the appropriate information and click 'Install Software' to begin the installation process.

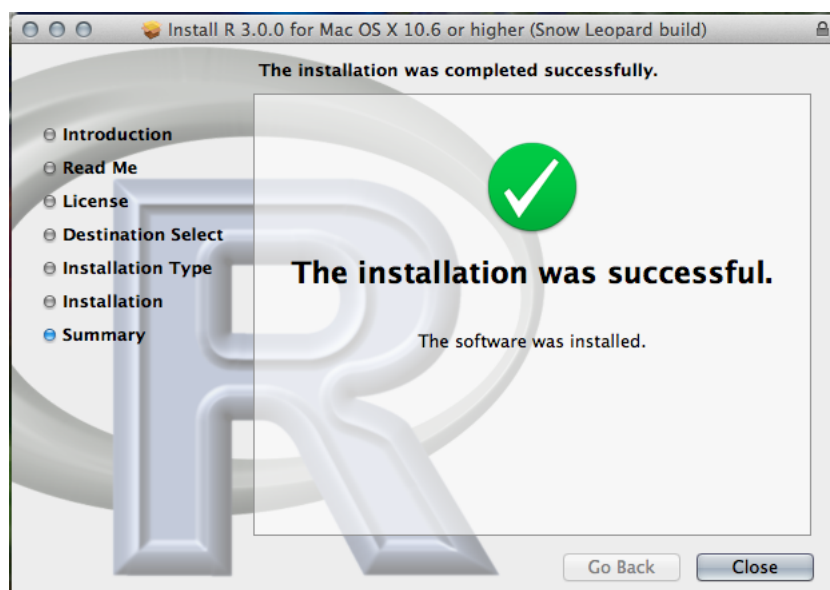


7. Once the installation process begins, wait a few moments for the packages to validate and install.

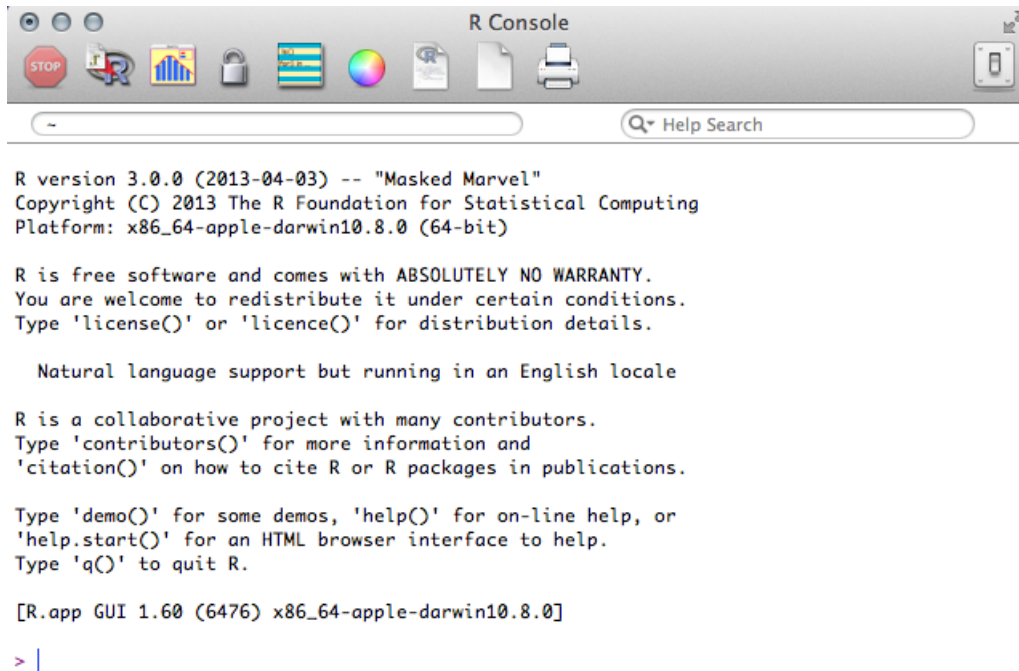




8. Once the installation completes successfully, click 'Close' to finish the installation process.



Out of the box, you can run an interactive R session in two separate ways: from the “gui” and from a terminal. To launch the R “gui”, simply go to your Applications folder in Finder and double-click R.app.



Once R is finished installing, you need to install the **rlecuyer** package. To install it from an interactive R session, simply start an R session and issue the command

```
1 install.packages("rlecuyer")
```

3.1.2 Compiling from Source

You can find R sources from <http://cran.r-project.org/sources.html>

Start by opening a terminal and navigate to the folder containing the R source package you just downloaded. You can extract the archive by executing, for example

```
tar zxvf R-3.0.0.tar.gz
```

From here, generally it should be enough to simply execute

```
./configure && make && make install
```

without problems.

3.2 Installing MPI

You have several options for installing OpenMPI on a Mac. You can install from [MacPorts](#), which is a relatively simple way to manage compiling/installing of many packages (such as OpenMPI). You can also compile from source.

Before beginning, make sure you have some “downtime” allotted, as the compilation will take upwards of a few hours for some machines.

3.2.1 Installing from a MacPorts

Arguably the easiest way to install OpenMPI for a Mac (that I'm aware of) is using [MacPorts](#), which is not unlike some source repositories for Linux. You can find information about installing MacPorts from [MacPorts installation page](#), maintained by the MacPorts project.

Once you have MacPorts installed, you can install openmpi from a terminal by issuing the command:

```
sudo port install openmpi
```

3.2.2 Compiling from Source

If you want to install OpenMPI from source (I don't really recommend this unless you think you have a good reason to), then the sources are available [here](#).

3.3 Installing pbdR Packages

Installing pbdR should go smoothly. The simplest way to install the packages is from an R terminal, which will manage dependencies for you much like the Mac App store.

3.3.1 Installing from CRAN

This is perhaps the simplest way to proceed, as R will handle any package dependency resolution for you. Simply start an R session (from the terminal¹, type R then press enter) and issue the command:

```
1 install.packages(<package>)
```

So for example, to install **pbdMPI**, you might execute:

```
1 install.packages(pbdMPI)
```

3.3.2 Installing from the Shell

If you have downloaded a pbdR (or other R) package, then installing from the shell simply amounts to issuing the command:

```
R CMD INSTALL <package>
```

So for example, to install **pbdMPI**, you might execute:

```
R CMD INSTALL pbdMPI_0.1-6.tar.gz
```

3.3.3 Installing from Github

CRAN policy is such that updates to packages can not be made too frequently. For this reason, the development versions of our packages will have bugfixes and new features much more quickly than CRAN versions.

¹Do *not* use the gui. See section [5.2](#) for details

The easiest way to install from github is using Hadley Wichkam's **devtools** package (which can be installed via `install.packages(devtools)`). Assuming you have this package installed, then from an R session, to install a pbdR package you would issue one of the following:

```
1 library(devtools)
2
3 install_github(repo="pbdMPI", username="RBigData")
4 install_github(repo="pbdSLAP", username="RBigData")
5 install_github(repo="pbdNCDF4", username="RBigData")
6 install_github(repo="pbdBASE", username="RBigData")
7 install_github(repo="pbdDMAT", username="RBigData")
8 install_github(repo="pbdDEMO", username="RBigData")
```

You can also install *really* new package builds, which will be very current in terms of features, but also bugs (or even complete package breakage). If you're sure you want these packages, then you can install them as follows:

```
1 # dev repo 1
2 install_github(repo="pbdMPI", username="snoweye")
3 install_github(repo="pbdSLAP", username="snoweye")
4 install_github(repo="pbdNCDF4", username="snoweye")
5 # dev repo 2
6 install_github(repo="SEXptools", username="wrathematics")
7 install_github(repo="pbdBASE", username="wrathematics")
8 install_github(repo="pbdDMAT", username="wrathematics")
9 install_github(repo="pbdDEMO", username="wrathematics")
```

4 Running pbdR Scripts

This information is covered in *much* more detail in the [pbdDEMO](#) vignette, and should not be considered a substitute. However, there are two key points one needs to understand in order to use pbdR tools. Namely,

- pbdR codes are written in Single Program/Multiple Data style
- pbdR codes are executed in batch

For full details, see the pbdDEMO package vignette.

Below is a simple pbdR script. This will help you know if things are installed properly or not. To understand what the script is doing, or to learn how to do much more substantial things, you should see the pbdDEMO package vignette.

```
1 library(pbdMPI, quiet = TRUE)
2 init()
3
4 x <- comm.rank()
5
6 comm.print(x, all.rank = TRUE)
7
8 finalize()
```

To run the script, you must do so in batch (i.e., non-interactively). First save its contents to the file `my_script.r`, and then open a terminal. On Mac, you should execute the command:

```
mpirun -np 2 Rscript my_script.r
```

5 Installation Problems

During the course of installation, you may run into unrecoverable issues. The pbdR team does not support MPI libraries or R core, so if you have problems during that portion of the installation phase, we probably can not directly help you. However, there are still many great resources at your disposal, maintained by those individual projects.

5.1 R and MPI

If you have problems installing or customizing R, see the *R Installation and Administration Manual* at <http://cran.r-project.org/doc/manuals/R-admin.html> for help.

If you are having trouble installing an MPI library, you should see that library's official documentation. For OpenMPI, see <http://www.open-mpi.org/community/help/> and for MPICH, see <http://www.mpich.org/documentation/guides/>.

For the remainder, we will be addressing installation issues with pbdR packages.

5.2 pbdR

This is a quick list of potential problems you could encounter when installing pbdR packages. For additional troubleshooting or installation options, each package has a vignette which may offer additional useful information.

- **When compiling pbdMPI from source**, you may be required to pass a configure argument at compile time. So for example, if you have OpenMPI installed and were installing from the command line, then you would issue the command:

```
R CMD INSTALL pbdMPI_0.1-6.tar.gz \
  --configure-args='--with-mpi-type=OPENMPI'
```

or if installing from R:

```
1 install.packages("pbdMPI", configure.args='--with-mpi-type=OPENMPI')
'
```

See the **pbdMPI** vignette for more details.

- **If you are installing on a cluster** where you must install on the login node which can not execute `mpirun`, then pass the install option `--no-test-load`. So for example, if installing from the command line, then you would issue the command:

```
R CMD INSTALL pbdMPI_0.1-6.tar.gz --no-test-load
```

or if installing from R:

```
1 install.packages("pbdMPI", INSTALL_opts='--no-test-load')
```

- **If you are installing binaries on MAC OS X**, do not use the gui. You can install from source using the gui, or you can install binaries (or from source) using the terminal. But you can not install binaries using the gui. So if you want to install binaries, you should open Finder, then navigate to **Applications/Utilities/** and select **Terminal**. Next, type **R** and press enter. Now try to install the packages.