pbdR Core Team

Setting up a pbdR Environment

Installing MPI, R, and pbdR

Setting Up a pbdR Environment

Installing MPI, R, and pbdR

Version 2.0

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 LATEX.

CONTENTS ii

Contents

1	Allocation	1
2	Quick Introduction 2.1 Installing R 2.2 Installing MPI 2.3 Installing pbdR Packages	1
3	Windows 3.1 Installing R 3.2 Installing Rtools 3.3 Installing MS-MPI 3.4 Installing pbdR Packages 3.4.1 Installing from Github 3.4.2 Installing from Downloaded Source	5 8 11 11
4	Running pbdR Scripts	13
5	Installation Problems 5.1 R and MPI	

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 (and Rtools for Windows); 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 additionally Rtools for Windows) 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

Windows users should install Microsoft MPI or MS-MPI (http://msdn.microsoft.com/en-us/library/bb524831(v=vs.85).aspx). Currently, pbdR is built with 'HPC Pack 2012 R2 MS-MPI Redistributable Package' which is available at http://http://www.microsoft.com/en-us/download/.

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 LATEX, 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

 $3 \quad WINDOWS$ 2 of 15

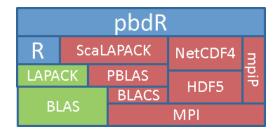


Figure 1: pbdR Relationships to Libraries

offers some insight into the package organization. See the pbdSLAP vignette for more details.

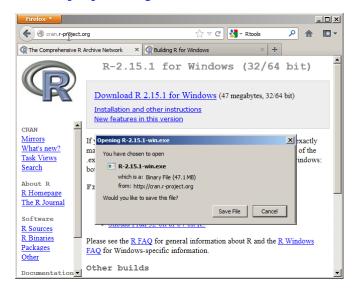
3 Windows

Officially, the pbdR team does not support gaming consoles (only kidding!). Jokes aside, it is possible to install a pbdR environment on Windows, but it is not necessarily the easiest. This guide will explain the basics of getting R, OpenMPI, and pbdR installed on your Windows system. The instructions and screenshots for this document are for version 2.15.1 of R, but later versions should be very similar, if not identical.

If you are completely new to R, then you may find the R for Windows FAQ useful. Additionally, there is also an 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

1. Download R: http://cran.r-project.org/bin/windows/base/

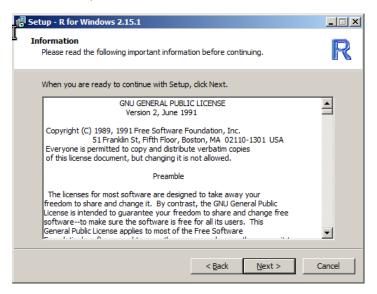


2. Open the saved file from 1 above to begin the installation. At the first setup screen, click 'Next' to continue.

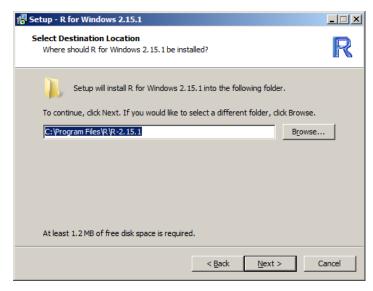
 $3 \quad WINDOWS$ 3 of 15



3. When prompted with the license, click 'Next' to continue.

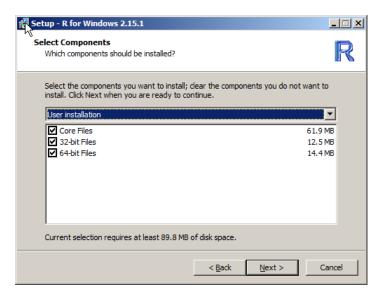


4. When prompted for the location to install R, we strongly encourage you to use the default. When you have made your decision, click 'Next'.

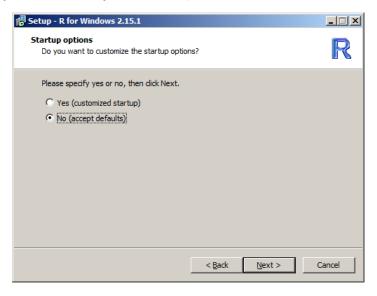


5. When prompted with the components to install, you should select a 'User installation'. Then click 'Next'.

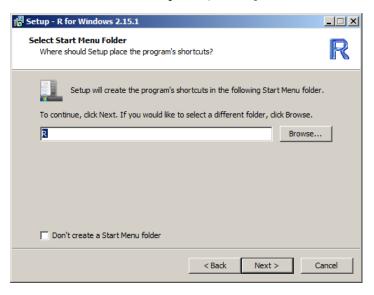
3 WINDOWS 4 of 15



6. When prompted with the option to alter the startup options, we suggest selecting No (accept defaults). When you have made your decision, click 'Next'.



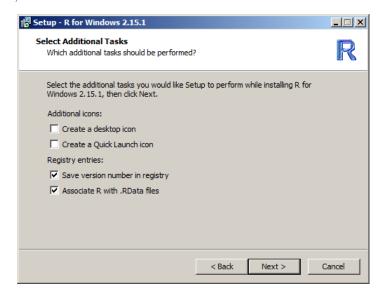
7. When prompted with the start menu folder options, make your choice and then click 'Next'.



8. When prompted with the additional tasks options, we suggest making sure that Save version number in registry and Associate R with .RData files are both checked. When you have

3 WINDOWS 5 of 15

made your decisions, click 'Next'.



9. To complete the R installation, select 'Finish'.



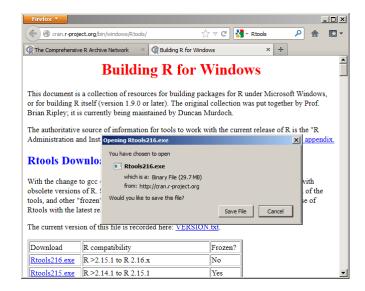
Once R is finished installing, you need to install the **rlecuyer** package. To install it from an interactive R session, simply start an R session and issue the command

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

3.2 Installing Rtools

1. Download Rtools: http://cran.r-project.org/bin/windows/base/

3 WINDOWS 6 of 15



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



3. When prompted with the license, click 'Next' to continue.

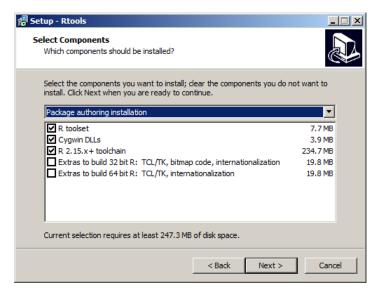


4. When prompted for the location to install R, we strongly encourage you to use the default. When you have made your decision, click 'Next'.

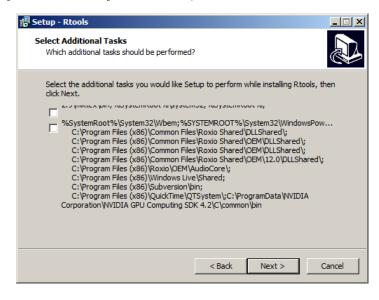
3 WINDOWS 7 of 15



5. When prompted with the components to install, you should select a 'User installation'. Then click 'Next'.

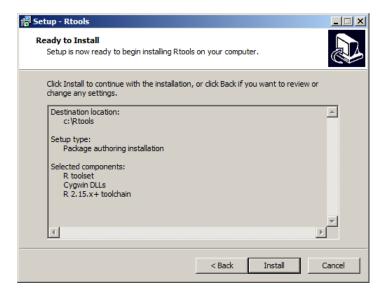


6. When prompted with the option to alter the startup options, we suggest selecting No (accept defaults). When you have made your decision, click 'Next'.



7. When prompted with the start menu folder options, make your choice and then click 'Next'.

3 WINDOWS 8 of 15



8. To complete the Rtools installation, select 'Finish'.



3.3 Installing MS-MPI

Before proceeding, please be aware that this installation requires Administrative privileges.

1. Download Microsoft MPI, MS-MPI, (HPC Pack 2012 R2 MS-MPI Redistributable Package) installers from: http://http://www.microsoft.com/en-us/download/.

 $3 \quad WINDOWS$ 9 of 15



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



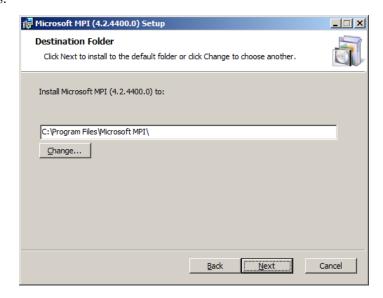
3. When prompted with the license, check "I accept the terms in the License Agreement" and then click 'Next' to continue.



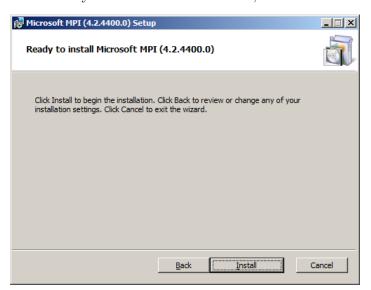
4. When prompted with the destination folder, click 'Next' to continue. We recommend you keep

3 WINDOWS 10 of 15

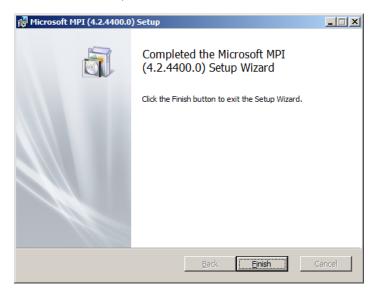
the default folders.



5. When prompted with the 'Ready to install Microsoft MPI', click 'Install' to continue.



6. To complete the MS-MPI installation, select 'Finish'.



3 WINDOWS 11 of 15

3.4 Installing pbdR Packages

You may install pbdR packages from source on Windows. We will present two approaches; the short way, installing from github using the **devtools** package, and a longer way, installing from a downloaded source file. However, do be aware that each of these methods requires the installation of the Rtools package from Section 3.2 (so that step cannot be skipped).

Finally, we note that it may not be possible to install the **pbdNCDF4** package on Windows. We have not tested this and, assuming it is possible, it would be very difficult to get NetCDF4 compiled in parallel first. If you have success installing this package on Windows, we would love to hear from you.

3.4.1 Installing from Github

This is probably the simplest method, assuming that you have Rtools installed and set up correctly. If Rtools is not in your PATH, then you may need to enter something like the following:

```
rtools <- "C:\\Rtools\\bin\\"
mingw <- "C:\\Rtools\\gcc-4.6.3\\bin\\"

PATH <- Sys.getenv("PATH")
### "C:\\Program Files\\Microsoft MPI\\Bin\\" should be in the PATH.

new.PATH <- paste(rtools, mingw, PATH, sep = ";")
Sys.setenv(PATH = new.PATH)

Sys.setenv(MPI_ROOT = "C:\\Program Files\\Microsoft MPI")</pre>
```

where the rtools and mingw directories are as they are on your machine. Also, "C:

Program Files

Microsoft MPI

Bin

" should be in the "PATH" and "MPI_ROOT" should be set to where MS-MPI installed.

Once that is settled, installing is fairly simple. You simply load the **devtools** package and install from our github repo as follows:

```
library(devtools)

install_github(repo="pbdMPI", username="RBigData")

install_github(repo="pbdSLAP", username="RBigData")

install_github(repo="pbdBASE", username="RBigData")

install_github(repo="pbdDMAT", username="RBigData")

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:

```
# dev repo 1
install_github(repo="pbdMPI", username="snoweye")
install_github(repo="pbdSLAP", username="snoweye")
```

 $3 \quad WINDOWS$ 12 of 15

```
# dev repo 2
install_github(repo="SEXPtools", username="wrathematics")
install_github(repo="pbdBASE", username="wrathematics")
install_github(repo="pbdDMAT", username="wrathematics")
install_github(repo="pbdDEMO", username="wrathematics")
```

3.4.2 Installing from Downloaded Source

1. To help simplify things, we offer a simple install script which makes managing the PATH slightly simpler. By default, this is for R version 3.0.1 and **pbdMPI** version 0.2-3. If you have a different version of R or want to install a different version of **pbdMPI**, simply change lines 4 and/or 5 of the install script to match your needs.

```
## Set environment variables.

SET R_VER=3.0.1

SET PBDMPI_VER=0.2-3

rem ### Set environment variables.

SET R_HOME=C:\Program Files\R\R-%R_VER%\

SET RHOME=%R_HOME%

SET RBIN=%R_HOME%

SET RBIN=%R_HOME% in\
SET MINGW=C:\Rtools\bin\
SET MINGW=C:\Rtools\bin\
SET MINGW=C:\Program Files\Microsoft MPI\

IF NOT DEFINED PATH_ORG SET PATH_ORG=%PATH%

SET PATH=%MPI_ROOT%Bin\;%RHOME%;%RBIN%;%RTOOLS%;%MINGW%;%PATH_ORG%

rem ### Build Windows binary.

R CMD INSTALL -build --html pbdMPI_%PBDMPI_VER%.tar.gz

R CMD INSTALL pbdMPI_%PBDMPI_VER%.zip
```

- 2. Open a command prompt either from the start menu, or by entering the command Windows key then R, and then entering cmd in the "run" dialog box.
- 3. Before proceeding further, it is probably a good idea to test the installation of MS-MPI. The following commands utilize MS-MPI to do some fairly trivial things (do not copy SHELL> if you are copying and pasting from the lines below):

```
SHELL> "C:\Program Files\Microsoft MPI\Bin\mpiexec" -np 2 hostname
.exe

SHELL> "C:\Program Files\R\R-3.0.1\bin\R" --vanilla --slave -e "ls
()"

SHELL> "C:\Program Files\R\R-3.0.1\bin\Rscript" --vanilla --slave
-e "ls()"
```

```
C:\Users\snoweye>"C:\Program Files\Microsoft MPI\Bin\mpiexec" -np 2 hostname.exe

WOLF_DELL
WOLF_DELL
C:\Users\snoweye>"C:\Program Files\R\R-3.0.1\bin\R" --vanilla --slave -e "ls()"
character(0)
C:\Users\snoweye>"C:\Program Files\R\R-3.0.1\bin\Rscript" --vanilla --slave -e "
ls()"
character(0)
C:\Users\snoweye>"C:\Program Files\R\R-3.0.1\bin\Rscript" --vanilla --slave -e "
ls()"
character(0)
C:\Users\snoweye>"
```

4. Download the source for **pbdMPI** package. Put it in the same directory as your build_pbdMPI.bat file, and then execute build_pbdMPI.bat from the command prompt to install the package.

```
👞 Administrator: Command Prompt
   \Users\snoweye>build_pbdMPI
  installing to library 'C:/Program Files/R/R-3.0.1/library
  installing *source* package 'pbdMPI' ...
 ** arch - i386
ygwin warning:
  MS-DOS style path detected: C:/PROGRA~1/R/R-30~1.1/etc/i386/Makeconf
  Preferred POSIX equivalent is: /cygdrive/c/PROGRA~1/R/R-30~1.1/etc/i386/Makeco
  CYGWIN environment variable option "nodosfilewarning" turns off this warning.
  Consult the user's guide for more details about POSIX paths:
    http://cygwin.com/cygwin-ug-net/using.html#using-pathnames
cho 'MPI HOME = C:\Program Files\Microsoft MPI\' > Makeconf
cho 'MPI_ROOT = C:\Program Files\Microsoft MPI\' >> Makeconf
     'MPI_ROOT_32 = C:\Program Files\Microsoft MPI\' >> Makeconf
'MPI_ROOT_64 = ' >> Makeconf
'MPI_INCLUDE = C:/PROGRA~1/MICROS~3/Inc/' >> Makeconf
echo
      'MPI_LIB = C:/PROGRA~1/MICROS~3/Lib/i386//msmpi.lib' >>
     'WIN_FLAGS = -DWIN -DMSMPI_NO_DEPRECATE_20' >> Makeconf
'WIN_MPI_TYPE = "MS-MPI"' >> Makeconf
echo
     'MSMPI_BIN = C:\Program Files\Microsoft MPI\Bin\' >> Makeconf
'MSMPI_INC = C:\Program Files\Microsoft MPI\Inc\' >> Makeconf
      'MSMPI_LIB32 = C:\Program Files\Microsoft MPI\Lib\i386\' >> Makeconf
```

5. If the process is done without errors, you can see the binary package is installed.

```
👞 Administrator: Command Prompt
                                                                                         kx_comm_base
    xx_comm_dist
                                                   html
    xx_comm_pairwise
                                                   html
    xx_comm_range
                                                   html
    xx_comm_sort
                                                   html
    xx_comm_stop_warning
xx_comm_timer
                                                   html
                                                   html
    xx_comm_which
                                                   html
    yy_api_apply
yy_api_task_pull
                                                   html
                                                   html
     zz_comm_internal
                                                   html
    zz_internal
zz_spmd_internal
                                                   html
                                                   html
   building package indices
   installing vignettes
    pbdMPI-guide.Rnw
   testing if installed package can be loaded
arch - i386
 ** arch - x64
 MD5 sums
 ackaged installation of 'pbdMPI' as pbdMPI_0.2-3.zip
 DONE (pbdMPI) installing to library 'C:/Program Files/R/R-3.0.1/library
 ackage 'pbdMPI' successfully unpacked and MD5 sums checked
```

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.

```
library(pbdMPI, quiet = TRUE)
init()

x <- comm.rank()

comm.print(x, all.rank = TRUE)

finalize()</pre>
```

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 command prompt. On Windows, you should execute the command: mpiexec.exe -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:

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~C\!M\!D~I\!N\!S\!T\!ALL~pbdMPI\_0.1-6.\,tar.\,gz~-\!-no-test-load
```

or if installing from R:

```
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.