A Quick Guide for the pbdMPI Package

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Warning: This document is written to explain the main functions of **pbdMPI** (Chen *et al.* 2012), version 0.1-1. Every effort will be made to ensure future versions are consistent with these instructions, but features in later versions may not be explained in this document.

Information about the functionality of this package, and any changes in future versions can be found on website: "Programming with Big Data in R" at http://r-pbd.org/.

1. Introduction

Our intent is to bring the most common parallel programming model from supercomputing, Single Program Multiple Data (SPMD), to R and enable distributed handling of truly large data. Consequently, **pbdMPI** is intended for batch mode programming with big data (pbd). Unlike **Rmpi** (Yu 2010), **snow** (Tierney et al. 2012), or **parallel** (R Core Team 2012), interactive mode is not supported. We think that interaction with a large distributed parallel computing platform is better handled with a client/server relationship, and we are developing other packages in this direction. **pbdMPI** simplifies MPI interaction, but leaves low and mid level functions available for advanced programmers. For example, it is easy to hand communicators to **pbdMPI** from other applications through MPI array pointers. This is intended for integration with other, possibly non-R, parallel software.

Under the SPMD parallel programming model, the identical program runs on every processor but typically works on different parts of a large data set, while communicating with other copies of itself as needed. Differences in execution stem from comm.rank, which is typically different on every processor. While on the surface this sounds complicated, after some experience and a new mindset, programming is surprisingly simple. There is no master. There is only cooperation among the workers. Although we target very large distributed computing platforms, SPMD works well even on small multicore platforms.

In the following, we list the main features of **pbdMPI**.

- 1. Under the SPMD batch programming model, a single program is written, which is spawned by mpirun. No spawning and broadcasting from within R are required.
- 2. S4 methods are used for most collective functions so it is easy to extend them for general R objects.
- 3. Default methods (like Robj functions in **Rmpi**) have homogeneous checking for data type so they are safe for general users.
- 4. The API in all functions is simplified, with all default arguments in control objects.
- 5. Methods for array or matrix types are implemented without serialization and un-serialization, resulting in faster communication than **Rmpi**.
- 6. Basic data types of integer, double and raw in **pbdMPI** are communicated without further checking. This is risky but fast for advanced programmers.
- 7. Character data type is serialized and communicated by raw type.

System requirements and installation of **pbdMPI** are described next. Section 2 gives a short example for comparing performance of **pbdMPI** and **Rmpi** (Yu 2010). In Section 3, a few

quick answers for questions are given. Section 4 provides settings for Windows environments. Finally, in Section 5, two examples from **parallel** are shown as SPMD **pbdMPI** programs.

1.1. System Requirements

pbdMPI requires MPI (http://en.wikipedia.org/wiki/Message_Passing_Interface). The package is mainly developed and tested under OpenMPI (http://www.open-mpi.org/) in xubuntu 11.04 (http://xubuntu.org/) and should also work with LAM/MPI (http://www.lam-mpi.org/) and MPICH2 (http://www.mcs.anl.gov/research/projects/mpich2/). In addition to unix, pbdMPI should also run under other operating systems such as Mac OS X with OpenMPI or Windows 7 with MPICH2 if MPI is installed and launched properly, although we have not tested on multiple machines yet. Please let us know about your experience.

For normal installation, see Sec. 1.2. To build as a static library, which may be required on some large systems, use

Shell Command

```
./configure --enable-static --prefix=${MPI_ROOT}
make
make install
```

where **--enable-static** can build a static library (optional), and \${MPI_ROOT} is the path to MPI root. Note that the static library is not necessary for **pbdMPI** but may avoid dynamic loading problems.

To make sure your MPI system is working, test with

Shell Command

```
mpiexec -np 2 hostname
```

This should list two host names where MPI jobs are running. Note to use hostname.exe with the extension on a Windows system.

1.2. Installation and Quick Start

One can download **pbdMPI** from CRAN at http://cran.r-project.org, and the intallation can be done with the following commands (using OpenMPI library)

Shell Command

```
tar zxvf pbdMPI_0.1-0.tar.gz
R CMD INSTALL pbdMPI
```

Further configure arguments include

Argument	Default
with-Rmpi-type	OPENMPI
with-Rmpi-include	\${MPI_ROOT}/include
with-Rmpi-libpath	\${MPI_ROOT}/lib
with-mpi	\${MPI_ROOT}

where \${MPI_ROOT} is the path to the MPI root. For non-default and unusual installations of MPI systems, the commands may be

Shell Command

See the package source file pbdMPI/configure for details.

One can get started quickly with **pbdMPI** by learning from the following six examples.

Shell Command

```
### At the shell prompt, run the demo with 2 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 2 Rscript -e "demo(allgather, 'pbdMPI', ask=F,echo=F)"
mpiexec -np 2 Rscript -e "demo(allreduce, 'pbdMPI', ask=F,echo=F)"
mpiexec -np 2 Rscript -e "demo(bcast, 'pbdMPI', ask=F,echo=F)"
mpiexec -np 2 Rscript -e "demo(gather, 'pbdMPI', ask=F,echo=F)"
mpiexec -np 2 Rscript -e "demo(reduce, 'pbdMPI', ask = F,echo=F)"
mpiexec -np 2 Rscript -e "demo(scatter, 'pbdMPI', ask=F,echo=F)"
```

1.3. Basic Steps

In the SPMD world, every processor is a worker, every worker knows about all the others, and each worker does its own job, possibly communicating with the others. Unlike the manager/workers style, SPMD is more likely to fully use the computer resources. The following shows typical basic steps of using **pbdMPI**.

- 1. Initialize. (init)
- 2. Read your portion of the data.
- 3. Compute. (send, recv, barrier, ...)
- 4. Communicate results among workers. (gather, allgather, reduce, allreduce, ...)
- 5. Finalize. (finalize)

In a given application, the Compute and Communicate steps may be repeated several times for intermediate results. The Compute and Communicate steps are more general than the "map" and "reduce" steps of the map-reduce paradigm but similar in spirit. One big difference is that the Communicate step may place the "reductions" on all processors rather than just one (the manager for map-reduce) for roughly the same time cost. With some experience, one can easily convert existing R scripts, and quickly parallelize serial code. **pbdMPI** tends to reduce programming effort, avoid complicated MPI techniques, and gain computing performance.

The major communication functions of **pbdMPI** and corresponding similar functions of **Rmpi** are listed in the following.

pbdMPI (S4)	Rmpi
allgather	mpi.allgather, mpi.allgatherv, mpi.allgather.Robj
allreduce	mpi.allreduce
bcast	<pre>mpi.bcast, mpi.bcast.Robj</pre>
gather	<pre>mpi.gather, mpi.gatherv, mpi.gather.Robj</pre>
recv	mpi.recv, mpi.recv.Robj
reduce	mpi.reduce
scatter	<pre>mpi.scatter, mpi.scatterv, mpi.scatter.Robj</pre>
send	mpi.send, mpi.send.Robj

1.4. More Examples

The package source files provide several examples based on **pbdMPI**, such as

Directory	Examples
pbdMPI/inst/examples/test_spmd/	main SPMD functions
<pre>pbdMPI/inst/examples/test_rmpi/</pre>	comparison to Rmpi
<pre>pbdMPI/inst/examples/test_parallel/</pre>	comparison to parallel
<pre>pbdMPI/inst/examples/test_performance/</pre>	performance testing
pbdMPI/inst/examples/test_s4/	S4 extension

2. Performance

There are more examples for testing performance in pbdMPI/inst/examples/test_rmpi. Here, we only show a simple comparison of pbdMPI to Rmpi. The two scripts are equivalent for pbdMPI and Rmpi. We run them with two processors and obtain computing times listed below.

Save the following script in demo_spmd.r and run it with two processors by

Shell Command

```
mpiexec -np 2 Rscript demo_spmd.r
```

to see the computing time on your platform.

pbdMPI R Script

```
### Save this script in "demo_spmd.r".
library(pbdMPI, quiet = TRUE)
init()

time.proc <- list()</pre>
```

```
time.proc$default <- system.time({
   for(i in 1:1000) y <- allgather(list(x = 1:10000))
   barrier()
})

time.proc$matrix <- system.time({
   for(i in 1:1000) y <- allgather(matrix(1:10000, nrow = 100))
   barrier()
})

comm.print(time.proc, quiet = TRUE)
finalize()</pre>
```

Save the following script in demo_rmpi.r and run with two processors by

Shell Command

```
mpiexec -np 2 Rscript demo_rmpi.r
```

to see the computing time on your platform.

Rmpi R Script

```
### Save this script in "demo_rmpi.r".
library(Rmpi)
invisible(mpi.comm.dup(0, 1))

time.proc <- list()
time.proc$Robj <- system.time({
   for(i in 1:1000) y <- mpi.allgather.Robj(list(x = 1:10000))
   mpi.barrier()
})

time.proc$matrix <- system.time({
   for(i in 1:1000) y <- mpi.allgather.Robj(matrix(1:10000, nrow = 100))
   mpi.barrier()
})

if(mpi.comm.rank(1) == 0) print(time.proc)
mpi.quit()</pre>
```

The following shows the computing time of the above two scripts on a single machine with two processors Intel(R) Core(TM) i5-2410M CPU @ 2.30 GHz, xubuntu 11.04 system, and OpenMPI 1.6. The **pbdMPI** is more efficient than **Rmpi** with list and matrix/array data structures.

R Output

```
>> Output from demo_spmd.r

$default

user system elapsed

1.680 0.030 1.706
```

```
$matrix
          system elapsed
   user
  0.950
          0.000
                   0.953
>> Output from demo_rmpi.r
$Robj
          system elapsed
   user
  2.960
          0.090
                   3.041
$matrix
         system elapsed
   user
                   3.147
  3.120
          0.030
```

3. FAQs

3.1. General

1. Q: Do I need MPI knowledge to run **pbdMPI**?

A: Yes, but only the big picture, not the details. We provide several examples in pbdMPI/inst/examples/test_spmd/ to introduce essential methods for learning MPI communication.

- 2. Q: Can I run **pbdMPI** on my laptop locally?
 - A: Sure, as long as you have an MPI system. You even can run it on 1 CPU.
- 3. Q: Does **pbdMPI** support Windows clusters?

A: Yes, the released binary currently supports OpenMPI and MPICH2. For other MPI systems, users have to compile from source.

- 4. Q: Can I run **pbdMPI** in OpenMPI and MPICH2 together?
 - **A:** No, you can have both OpenMPI and MPICH2 installed in your OS, but you are only allowed to run **pbdMPI** with one MPI system. Just pick one.
- 5. Q: Does **pbdMPI** support any interactive mode?
 - **A:** No, but yes. **pbdMPI** only considers batch execution and aims for programming with big data that do not fit on desktop platforms. We think that interaction with big data on a big machine is better handled with a client/server interface, where the server runs SPMD codes on big data and the client operates with reduced data representations.

If you really need an interactive mode, such as for debugging, you can utilize **pbdMPI** scripts inside **Rmpi**. **Rmpi** mainly focuses on Manager/Workers computing environments, but can run SPMD codes on workers only with a few adjustments. See the "Programming with Big Data in R" website for details at http://r-pbd.org/.

Note that **pbdMPI** uses communicators different from **Rmpi**. Be sure to free the memory correctly for both packages before quitting. finalize(mpi.finalize = FALSE) can free the memory allocated by **pbdMPI**, but does not terminate MPI before calling mpi.quit of **Rmpi**.

6. Q: Can I write my own collective functions for my own data type?

A: Yes, S4 methods allow users to add their own data type, and functions. Quick examples can be found in pbdMPI/inst/examples/test_s4/.

3.2. Programming

1. Q: Can I run task jobs by using **pbdMPI**?

A: Yes, it is relatively straightforward for parallel tasks. Neither extra automatic functions nor further command/data communication is required. In other words, SPMD is easier for Monte Carlo, bootstrap, MCMC simulation and statistical analysis for ultralarge datasets.

Example 1:

SPMD R Script

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

id <- get.jid(total.tasks)

### Using a loop
for(i in id){
    # put independent task i script here
}

### or using apply-like functions.
lapply(id, function(i){
    # put independent task i script here.
})

finalize()</pre>
```

Note that id gets different values on different processors, accomplishing total.tasks across all processors. Also note that any data and partial results are not shared across the processors unless communicated.

Example 2:

SPMD R Script

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

### Directly using a loop
for(i in 1:total.tasks){
  if(i %% comm.size() == comm.rank()){
    # put independent task i script here
}
}

### or using apply-like function.
```

```
lapply(1:total.tasks, function(i){
  if(i %% comm.size() == comm.rank()){
    # put independent task i script here.
}
})
finalize()
```

- 2. Q: What if I want to run task push or pull by using **pbdMPI**?
 - **A:** No problem. As in the two preceding examples, task push or pull can be done in the same way by using rank 0 as the manager and the other ranks as workers. However, we do not recommend it except perhaps for inhomogeneous computing environments.
- 3. Q: Are S4 methods more efficient?
 - A: Yes and No. S4 methods are a little less efficient than using switch ... case ... in C, but most default methods use raw with un- and serialize which may cost 3-10 times more than using integer or double. Instead of writing C code, it is easier to take advantage of S4 methods to extend to general R objects (matrix, array, list, data.frame, and class ...) by communicating with basic data types (integer and double) and avoiding serialization.
- 4. Q: Can **pbdMPI** take or export communicators?
 - A: Yes, the physical memory address is set to the variable .__MPI_APTS__ in the .GlobalEnv through a call to init(). The variable points to a structure containing MPI structure arrays preallocated while pbdMPI is loaded. pbdMPI/src/pkg_* provides a mechanism to take or export external/global variables at the C language level.

3.3. MPI Errors

1. Q: If installation fails with

Error Message

```
Error in dyn.load(file, DLLpath = DLLpath, ...) :
  unable to load shared object '/.../pbdMPI/libs/pbdMPI.so':
  libmpi.so: cannot open shared object file: No such file or
      directory
```

A: OpenMPI may not be installed in the usual location, so the environment variable LD_LIBRARY_PATH should be set to the libmpi.so path, such as

Shell Command

```
export LD_LIBRARY_PATH=/usr/local/openmpi/lib:$LD_LIBRARY_PATH
```

where /usr/local/openmpi/lib should be replaced by the path to libmpi.so. Or, use LD_PRELOAD to preload the MPI library if the library name is not conventional, such as

Shell Command

```
export LD_PRELOAD=/usr/local/openmpi/lib/libmpi.so:$LD_PRELOAD
```

Another solution may be to use the unix command ldconfig to setup the correct path.

2. **Q: pbdMPI** installs successfuly, but fails at initialization when calling the function init() with error message

Error Message

```
/usr/lib/R/bin/exec/R: symbol lookup error:
/usr/lib/openmpi/lib/openmpi/mca_paffinity_linux.so: undefined
    symbol:
mca_base_param_reg_int
```

A: The linked library at installation may be different from the runtime library, especially when your system has more than one MPI systems. Since the library at installation is detected by autoconf (configure) and automake (Makevars), it can be linked with OpenMPI library, but MPICH2 or LAM/MPI is searched before OpenMPI according to \$PATH.

Solutions:

- Check which MPI system is your favorite to call. If you use OpenMPI, then you have to link with OpenMPI. Similarly, for MPICH2.
- Or, only kepp the MPI system you do like and drop others.
- Use --with-Rmpi-type to specify the MPI type.
- Use --with-Rmpi-include and --with-Rmpi-libpath to specify the right version.
- 3. Q: (Linux) If OpenMPI mpiexec fails with

Error Message

A: The linked MPI library libmpi.so may be missing or have a different name. Open-MPI builds shared/dynamic libraries by default and the target file libmpi.so is used by pbdMPI/src/spmd.c through #include <dlfcn.h> and dlopen(...) in the file pbdMPI/src/pkg_dl.c.

Solutions:

- Check if the path and version of libmpi.so are correct. In particular, one may have different MPI systems installed.
- When linking with libmpi.so in OpenMPI, one must run/load **pbdMPI** with OpenMPI's libmpi.so. The same for LAM/MPI and MPICH2.

- Use export LD_PRELOAD=\$PATH_TO_libmpi.so.* in command mode.
- Use the file /etc/ld.so.conf and the command ldconfig to manage personal MPI installation.
- Or, recompile OpenMPI with a static library, and use libmpi.a instead.
- 4. Q: (Windows) If OpenMPI mpiexec fails with

Error Message

```
ORTE_ERROR_LOG: Error in file ..\..\openmpi-1
.6\orte\mca\ess\hnp\ess_hnp_module.c at line 194
...
ORTE_ERROR_LOG: Error in file ..\..\openmpi-1
.6\orte\runtime\orte_init.c at line 128
...
```

A: Check if the network is unplugged, the network should be "ON" even on a single machine. At least, the status of network interface should be correct.

5. Q: For MPICH2 users, if installation fails with

Error Message

```
/usr/bin/ld: libmpich.a(comm_get_attr.o): relocation R_X86_64_32 against `MPIR_ThreadInfo' can not be used when making a shared object; recompile with -fPIC libmpich.a: could not read symbols: Bad value collect2: ld returned 1 exit status
```

A: MPICH2 by default does not install a shared library which means libmpich.so is missing and **pbdMPI** trys to link with a static library libmpich.a instead. Try to recompile MPICH2 with a flag -enable-shared and reinstall **pbdMPI** again.

4. Windows Systems

Currently, pbdMPI supports Windows with MPICH2 (http://www.mcs.anl.gov/research/projects/mpich2/). The binary installations of both MPI systems are available from the website. mpich2-1.4.1p1-win-ia32.msi is for 32-bits and mpich2-1.4.1p1-win-x86-64.msi is for 64-bits. The installation is easily done with a few clicks. The default environment and path are recommended.

For running MPI and R, users need to set PATH to the mpiexec.exe and Rscript.exe. By default,

Shell Command

```
### Under command mode, or save in a batch file.
SET R_HOME=C:\Program Files\R\R-2.15.1
SET MPI_ROOT=C:\Program Files\MPICH2
SET PATH=%MPI_ROOT%\bin\;%R_HOME%\bin\;%PATH%
```

is for the 64-bit MPICH2, but replace

Shell Command

```
SET MPI_ROOT=C:\Program Files (x86)\MPICH2
```

for the 32-bit MPICH2.

4.1. Install from Binary

The binary packages of **pbdMPI** are available on the website: "Programming with Big Data in R" at http://r-pbd.org/. Note that different MPI systems require different binaries. The binary can be installed by

Shell Command

```
R CMD INSTALL pbdMPI_0.1-0.zip
```

As on Unix systems, one can start quickly with **pbdMPI** by learning from the following demos. There are six basic examples.

Shell Command

```
### Run the demo with 2 processors by
mpiexec -np 2 Rscript.exe -e "demo(allgather,'pbdMPI',ask=F,echo=F)"
mpiexec -np 2 Rscript.exe -e "demo(allreduce,'pbdMPI',ask=F,echo=F)"
mpiexec -np 2 Rscript.exe -e "demo(bcast,'pbdMPI',ask=F,echo=F)"
mpiexec -np 2 Rscript.exe -e "demo(gather,'pbdMPI',ask=F,echo=F)"
mpiexec -np 2 Rscript.exe -e "demo(reduce,'pbdMPI',ask=F,echo=F)"
mpiexec -np 2 Rscript.exe -e "demo(scatter,'pbdMPI',ask=F,echo=F)"
```

Warning: Note that spacing inside demo is not working for Windows systems and Rscript.exe should be evoked rather than Rscript.

4.2. Build from Source

Warning: This section is only for building binary in 32- and 64-bit Windows system. A more general way can be found in the file pbdMPI/INSTALL.win.

Make sure that R, Rtools, and MINGW are in the PATH. See details on the website "Building R for Windows" at http://cran.r-project.org/bin/windows/Rtools/. But, if both 32-and 64-bits MPICH2 are installed, two different environment variables MPI_ROOT_32 and MPI_ROOT_64 need to be set for building binaries.

For example, the minimum requirement may be

Shell Command

```
### Under command mode, or save in a batch file.
SET R_HOME=C:\Program Files\R\R-2.15.1
SET RTOOLS=C:\Rtools\bin\
SET MINGW=C:\Rtools\gcc-4.6.3\bin
SET PATH=%R_HOME%;%R_HOME%\BIN\;%RTOOLS%;%MINGW%;%PATH%
SET MPI_ROOT_64=C:\Program Files\MPICH2
SET MPI_ROOT_32=C:\Program Files (x86)\MPICH2
```

With a correct PATH, one can use the R commands to install/build the **pbdMPI**:

Shell Command

```
### Under command mode, build and install the binary.
tar zxvf pbdMPI_0.1-0.tar.gz
R CMD INSTALL --build pbdMPI
R CMD INSTALL pbdMPI_0.1-0.zip
```

5. SPMD in Examples from package parallel

We demonstrate how a simple script from **parallel** can be written in batch by using **pbdMPI**. Each time, we first give the version using **parallel** followed by the version using **pbdMPI**. All codes are available in pbdMPI/inst/examples/test_parallel/.

Example 1: (mclapply() originates in multicore (Urbanek 2011)) Save the following script in a file and run with

Shell Command

```
Rscript 01_mclapply_par.r
```

to see the computing time on your platform.

multicore R Script

```
### File Name: 01_mclapply_par.r
library(parallel)

system.time(
  unlist(mclapply(1:32, function(x) sum(rnorm(1e7))))
)
```

Now save this script in a file and run with

Shell Command

```
mpirun -np 2 Rscript 01_mclapply_spmd.r
```

to see the computing time on your platform.

SPMD R Script

```
### File Name: 01_mclapply_spmd.r
library(pbdMPI, quiet = TRUE)
init()

time.proc <- system.time({
  id <- get.jid(32)
  ret <- unlist(lapply(id, function(i) sum(rnorm(1e7))))
  ret <- allgather(ret, unlist = TRUE)
})
comm.print(time.proc)

finalize()</pre>
```

The following shows the computing time of the above codes on a single local machine with two cores Intel(R) Core(TM) i5-2410M CPU @ 2.30 GHz, xubuntu 11.04 system, and OpenMPI 1.6. There is not much communication latency in this example since all computings are on one "node" which is also a limitation of **parallel**.

R Output

```
>> Test ./01_mclapply_par.r
   user system elapsed
16.800   0.570   17.419

>> Test ./01_mclapply_spmd.r
COMM.RANK = 0
   user system elapsed
17.130   0.460   17.583
```

Example 2: (parMM() originates in **snow** (Tierney *et al.* 2012)) Save the following code in a file and run with two processors

Shell Command

```
Rscript 02_parMM_par.r
```

to see the computing time on your platform.

snow R Script

```
### File Name: 02_parMM_par.r
library(parallel)
cl <- makeCluster(2)

splitRows <- function (x, ncl){
    lapply(splitIndices(nrow(x), ncl), function(i) x[i, , drop = FALSE])
}
parMM <- function (cl, A, B){
    do.call(rbind, clusterApply(cl, splitRows(A, length(cl)),
        get("%*%"), B))
}

set.seed(123)
A <- matrix(rnorm(1000000), 1000)
system.time(replicate(10, A %*% A))
system.time(replicate(10, parMM(cl, A, A)))

stopCluster(cl)</pre>
```

Now save this script in a file and run with

Shell Command

```
mpirun -np 2 Rscript 02_parMM_spmd.r
```

to see the computing time on your platform.

SPMD R Script

```
### File Name: O2_parMM_spmd.r
library(pbdMPI, quiet = TRUE)
init()

set.seed(123)
x <- matrix(rnorm(1000000), 1000)

parMM.spmd <- function(x, y){
  id <- get.jid(nrow(x))
  do.call(rbind, allgather(x[id,] %*% y))
}
time.proc <- system.time(replicate(10, parMM.spmd(x, x)))
comm.print(time.proc)

finalize()</pre>
```

The following shows the computing time of the above code on a single machine with two processors Intel(R) Core(TM) i5-2410M CPU @ 2.30 GHz, xubuntu 11.04 system, and OpenMPI 1.6. **pbdMPI** performs better than **snow** in this example even without communication over network.

R Output

```
>> Test ./02_parMM_par.r
    user system elapsed
12.460     0.170     12.625
    user system elapsed
1.780     0.820     10.095

>> Test ./02_parMM_spmd.r
COMM.RANK = 0
    user system elapsed
8.84     0.42     9.26
```

References

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