A Quick Guide for the pbdMPI Package

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This document is written to explain the main functions of **pbdMPI** (?), version 0.3-0. 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** (?), **snow** (?), or **parallel** (?), 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** (?). In Section 8, a few quick answers for questions are given. Section 7 provides settings for Windows environments. In Section 3, two examples from **parallel** are shown as SPMD **pbdMPI** programs. Section 4 discusses long vector support and communication in **pbdMPI** as an extension from R. Finally, in Section 5, some simple input and output methods between regular text/csv/csv2 files and data.frame are introduced.

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/). The package should also work with MPICH2 (http://www.mcs.anl.gov/research/projects/mpich2/) and Microsoft MPI or MS-MPI (http://msdn.microsoft.com/en-us/library/bb524831(v=vs.85).aspx). In addition to unix, pbdMPI should also run under other operating systems such as Mac OS X with OpenMPI or Windows 7 with MS-MPI 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 https://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-mpi-type	OPENMPI
with-mpi-include	\${MPI_ROOT}/include
with-mpi-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
podivii (54)	1011p1
allgather	<pre>mpi.allgather, mpi.allgatherv, mpi.allgather.Robj</pre>
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	<pre>mpi.send, mpi.send.Robj</pre>

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
<pre>pbdMPI/inst/examples/test_s4/</pre>	S4 extension
<pre>pbdMPI/inst/examples/test_cs/</pre>	client/server examples
<pre>pbdMPI/inst/examples/test_long_vector/</pre>	long vector examples

where test_long_vector/ requires to recompile with setting

```
pkg_constant.h

#define MPI_LONG_DEBUG 1
```

in pbdMPI/src/pkg_constant.h. See Scetion 4 for details.

Further examples can be found at including:

• "Introduction to distributed computing with pbdR at the UMBC High Performance Computing Facility (Technical Report, 2013)." (?)

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.

$\mathbf{pbdMPI} \ \mathrm{R} \ \mathrm{Script}$

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

time.proc <- list()
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({</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
  user
         system elapsed
          0.000
                   0.953
  0.950
>> Output from demo_rmpi.r
$Robj
         system elapsed
   user
  2.960
                   3.041
          0.090
$matrix
         system elapsed
  user
                   3.147
  3.120
          0.030
```

3. 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 (?)) 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
suppressMessages(library(pbdMPI, quietly = 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)</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 (?))

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: O2_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
suppressMessages(library(pbdMPI, quietly = 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
          system
                 elapsed
   user
  1.780
           0.820
                   10.095
>> Test ./02_parMM_spmd.r
COMM.RANK = 0
                 elapsed
   user
          system
   8.84
            0.42
                     9.26
```

4. Long Vector and 64-bit for MPI

We add new supports for long vector and communications based on MPI functions to **pbdMPI** since version 0.2-1.

4.1. Long Vector for MPI

The current R (3.1.0) uses C structure to extend 32-bit length limitation ($2^{31}-1=2147483647$ defined as R_SHORT_LEN_MAX) to 52-bit length ($2^{51}-1=4503599627370496$ defined as R_XLEN_T_MAX). In general, this is more portable and extensible when 128-bit integer comming on (who know when the day comes ...) However, a vector with elements larger than $2^{31}-1$ needs extra effort to be accessed in R. See "R Internals" for details.

The reason is that an integer is 4 bytes in both of x86_64 system (64-bit) and i386 system (32-bit). Since the capacity of current machine and performance issues, there is no benefit to use 8 bytes for integer. In x86_64 system, computers or compilers use either long or long long for pointer address which is in size_t for unsigned address or in ptrdiff_t for signed address. For example, in GNU C (gcc), the flag -m64 is to use 4 bytes for int and 8 bytes for long in x86_64 system.

Therefore, the question is what are the differences of 64-bit and 32-bit system? One of them is "pointer size" which is 8 bytes in x86_64 machine and it is 4 bytes in i386 machine. This allows computer to lengthen memory and disk space. Note that address is indexed by long or long long which is no confilict with integer size, and 4 bytes integer is efficient and safe enough for general purpose. For example, double *a is a pointer (a) pointing to a real scaler (*a), but the pointer's address (&a) is in size_t (long or long long) which is 8 bytes in x86_64 system and is 4 bytes in i386 system.

To deal with long vector, **pbdMPI** uses the same framework as R to build up MPI collective functions. **pbdMPI** follows R's standard to assume a vector normally has length smaller than R_SHORT_LEN_MAX which can be handled by most 32-bit functions. If the vector length is greater than R_SHORT_LEN_MAX, then R names this as long vector which also has the maximum R_XLEN_T_MAX. The vector length is stored in type R_xlen_t. The R_xlen_t is long if LONG_VECTOR_SUPPORT is defined, otherwise it is int. R provides several C macro to check, access, and manipulate the vector in VECSXP or general SEXP. See Rinternals.h for details.

The **pbdMPI** first checks if the data size for communication is greater than SPMD_SHORT_LEN_MAX or not. If the data is long vector, then **pbdMPI** evokes collective functions to send/receive

¹ Is there a way to have 8 bytes integer? The answer is that it is dependent on compiler.

chunk of data partitioned by SPMD_SHORT_LEN_MAX until all chunks are all received/sent. For some MPI collective functions such as allgather() and gather(), extra space may be allocated for receiving chunks, then the chunks are copied to right memory address by the rank of communicator from the extra space to the receiving buffer.

The reason is that most MPI collective functions rely on arguments for indexing buff types and counting buffer sizes where the types and sizes are both in int. SPMD_SHORT_LEN_MAX is defined in pbdMPI/src/spmd.h and usually is equal to R_SHORT_LEN_MAX. Developers may want to use shorter length (such as SPMD_INT8_LEN_MAX which is $2^7 - 1 = 127$) for testing without a large memory machine or for debugging without recompiling R with shorter R_SHORT_LEN_MAX.

In **pbdMPI**, the implemented MPI collective functions for long vector are bcast(), allreduce(), reduce(), send(), recv(), isend(), irecv(), allgather(), gather(), and scatter(). The other MPI collective functions are "NOT" implemented due to the complexity of memory allocation for long vector including allgatherv(), gatherv(), scatterv(), sendrecv(), and sendrecv.replace().

Further, **pbdMPI** provides a way to mimic long vector support. Users can set

pkg_constant.h

```
#define MPI_LONG_DEBUG 1
```

in pbdMPI/src/pkg_constant.h to turn on debugging mode and recompile pbdMPI. Then, run examples in pbdMPI/inst/examples/test_long_vector/ to see how the mimic long vectors are communicated between processors. Also, users can also adjust the length limit of mimic long vector (buffer size) by changing

spmd.h

```
#define SPMD_SHORT_LEN_MAX R_SHORT_LEN_MAX
```

in pbdMPI/src/spmd.h.

4.2. 64-bit for MPI

The remaining question is that does MPI library support 64-bit system? The answer is yes, but users may need to recompile MPI libraries for 64-bit support. The same way as R to enable 64-bit system that MPI libraries may have 8 bytes pointer in order to communicate larger memory or disk space.²

For example, the OpenMPI provides next to check if 64-bit system is used.

Shell Command

```
ompi_info -a | grep 'int.* size: '
```

If the output is

Shell Command

C int size: 4

² http://wiki.chem.vu.nl/dirac/index.php/How_to_build_MPI_libraries_for_64-bit_integers.

```
C pointer size: 8
Fort integer size: 8
Fort integer1 size: 1
Fort integer2 size: 2
Fort integer4 size: 4
Fort integer8 size: 8
Fort integer16 size: -1
```

then the OpenMPI supports 64-bit system.³ Otherwise, users may use the next to reinstall OpenMPI as

Shell Command

```
./configure --prefix=/path_to_openmpi \
    CFLAGS=-fPIC \
    FFLAGS="-m64 -fdefault-integer-8" \
    FCFLAGS="-m64 -fdefault-integer-8" \
    CFLAGS=-m64 \
    CXXFLAGS=-m64
```

and remember to reinstall **pbdMPI** as well.

Note that 64-bit pointer may only provide larger size of data, but may degrade hugely for other computing. In general, communication with a large amount of data is a very bad idea. Try to redesign algorithms to communicate lightly such as via sufficient statistics, or to rearrange and load large data partially or equally likely to every processors.

5. Simple Input and Output

We add new supports simple data input and output for basic CSV and text files to **pbdMPI** since version 0.2-2.

Two quick demos can simply explain how a dataset can be input and output via **pbdMPI** functions comm.write.table() and comm.read.table(). The first is

Shell Command

```
### Run the demo with 4 processors by mpiexec -np 4 Rscript -e "demo(simple_io,'pbdMPI',ask=F,echo=F)"
```

The demo utilizing iris data (?) to show simple input and output functions of **pbdMPI** and is summarized as in next.

- 150 rows of iris are divided in 4 processors, and processors own 37, 37, 38, and 38 rows of iris as a gbd row-block format. i.e. Rank 0 owns row 1 to 37, rank 1 owns row 38 to 74, and so on.
- A text file "iris.txt" is dumped via comm.write.table() which sequentially append processor owned row blocks.
- comm.read.table() then reads the text file back in memory, and again in a gbd row-block format.

³ The C integer is still in 4 bytes rather than 8 bytes.

Note that <code>comm.read.table()</code> may read a first few lines to predetermine how many lines of the file to read in. This is an approximation and results in unbalance data across processors. In particular, either the highest order rank may own the largest portion of whole dataset, or several higher order ranks may own zero row. So, a call <code>comm.load.balance()</code> within <code>comm.read.table()</code> is to move rows across processors if necessary. Basically, the reading steps are described as in the next.

- 1. If file size were less than 5MB, then rank 0 would read in the whole file and scatter rows to other ranks.
- 2. If file size were large than 5MB, then rank 0 would read in the first 500 lines and estimate total number of records in the file. All ranks sequentially read in the designated records.
- 3. Call comm.load.balance() to balance the data.

The file size limit is controlled by .pbd_env\$SPMD.IO\$max.file.size, and the first few line limit is controlled by .pbd_env\$SPMD.IO\$max.test.lines. Further, users can specify options nrows and skip to comm.read.*() to manually read the file and call comm.load.balance() later if needed.

There are several way to distributed or balance data among processors. Currently **pbdMPI** supports 3 formats: block, block0, and block.cyclic. In the above demo, the 150 rows are mainly distributed in (37, 37, 38, 38) which is a block format. The second demo shows how to load balance between different formats next.

Shell Command

```
### Run the demo with 4 processors by mpiexec -np 4 Rscript -e "demo(simple_balance,'pbdMPI',ask=F,echo=F)"
```

In the block0, the iris is distributed as (38, 38, 37, 37) row-bock of each processor. In the block.cyclic, the iris is distributed as (38, 38, 38, 36) row-bock of each processor. i.e. Each cycle has 38 rows and one cycle per processor.

See **pbdDEMO** vignettes (?) for more details about "block-cyclic" and "gbd".

6. Simple Pairwise Evaluation

We build some utilities for pairwise evaluation to **pbdMPI** since version 0.2-3.

Evaluating a function on any two data points is a common problems, such as distance, pairwise comparison, and multiple testing problems. Useful functions to solve those problems are

- comm.as.gbd(): This function is to turn a common matrix (in all ranks) to a gbd matrix in row major blocks. For example, one may read in data from one rank, then utilizes this function to redistribute data with load balance of all ranks. This is an alternative way to Section 5, but more efficient for small size of data.
- comm.allpairs(): This function is mainly to provide indices for all pairs of N data points. It returns a two columns (i, j) gbd matrix in row major blocks. For example, one may want to evaluate all N^2 pairs of the N data points. However, in distance context, it provides only indices as in lower-triangular matrix (ordered by row major).

- comm.dist(): This function is to compute distance (lower-triangular only) of N data points as usual dist() function, but evaluated on a gbd matrix in row major blocks. The returning can be a common distance matrix (only good for small dataset), or a 3 columns gbd matrix in row major blocks. The columns are i, j, and the value of pair (i, j).
- comm.pairwise(): This functions is a general extension composed of three functions above that allows users to provide a function FUN to evaluate on pairs of data. For example, a distance between two data points x and y can be computed via original dist() function. So, it can be wrapped as

R Script

```
dist.pair <- function(x, y, ...){
  as.vector(dist(rbind(x, y), ...))
}</pre>
```

for the FUN option of comm.pairwise().

This function is also useful for cases that measure of pair (i, j) differs to that of pair (j, i), i.e. non-symmetric measure. If order is matter, then the FUN can be evaluated via the options either pairid.gbd which can be user defined or simply symmetric = FALSE.

Also, we provide some examples in man page. A demo verifies these functions in different ways.

Shell Command

```
### Run the demo with 4 processors by mpiexec -np 4 Rscript -e "demo(simple_pairs,'pbdMPI',ask=F,echo=F)"
```

See **pbdDEMO** vignettes (?) for more statistical examples.

7. Windows Systems (MS-MPI)

Originally, **pbdMPI** (later than version 0.2-3 but only up to version 0.3-1) supports Windows with Microsoft MPI or MS-MPI (http://msdn.microsoft.com/en-us/library/bb524831(v=vs.85).aspx). **pbdMPI** was built with 'HPC Pack 2012 R2 MS-MPI Redistributable Package' which is available at http://http://www.microsoft.com/en-us/download/. The installation (MSMPISetup.exe) is easily done with a few clicks provided some service packs and Visual C++ runtime are installed correctly. The default environment and path are recommended for installation.

Currently, **pbdMPI** (later than version 0.3-2) supports Windows with Microsoft MPI or MS-MPI version 7.1 (https://www.microsoft.com/en-us/download/details.aspx?id=52981). Note that this is only a SDK development library which does not contain any MPI executable file such as mpiexec.exe. This is only for compiling and linking the **pbdMPI** with MPI library. However, you will still need 'MS-MPI Redistributable Package' to have a mpiexec.exe to run MPI programs or **pbdMPI** scripts.

The difference of default installation between the SDK library and 'Redistributable Package' are

- the location of MPI header file, and
- the location of the default installation.

The include path is changed from (Redistributable)

Shell Command

```
MPI_INCLUDE = ${MPI_ROOT}Inc/
```

to (SDK)

Shell Command

```
MPI_INCLUDE = ${MPI_ROOT}Include/
```

These are used by pbdMPI/src/Makevars.win. The default installation is changed from (Redistributable)

Shell Command

```
SET MPI_HOME=C:\Program Files\Microsoft MPI\
```

to (SDK)

Shell Command

```
SET MPI_HOME=C:\Program Files (x86)\Microsoft SDKS\MPI\
```

These are supposed to be set in a batch file.

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-3.0.1\

SET MPI_HOME=C:\Program Files\Microsoft MPI\

SET PATH=%MPI_HOmE%bin\;%R_HOME%bin\;%PATH%
```

Note that the installation (MSMPISetup.exe) may set several environmental variables including

- MSMPI_BIN for mpiexec.exe and other executable files,
- MSMPI_INC for header files such as mpi.h,
- MSMPI_LIB32 for 32 bits static libraries such as msmpi.lib, and
- MSMPI_LIB64 for 64 bits static libraries.

These should be useful to verify via R command Sys.getenv().

7.1. Install from Binary

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

Shell Command

```
R CMD INSTALL pbdMPI_0.2-3.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.

7.2. 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.

Make sure that R, Rtools, and MINGW are in the PATH. See details on the website "Building R for Windows" at https://cran.r-project.org/bin/windows/Rtools/. The environment variable MPI_HOME needs to be set for building binaries.

For example, the minimum requirement (for Rtools32 or earlier) may be

Shell Command

```
### Under command mode, or save in a batch file.
SET R_HOME=C:\Program Files\R\R-3.0.1\
SET RTOOLS=C:\Rtools\bin\
SET MINGW=C:\Rtools\gcc-4.6.3\bin\
SET MPI_HOME=C:\Program Files\Miscrosoft MPI\
SET PATH=%MPI_HOME%bin;%R_HOME%;%R_HOME%bin;%RTOOLS%;%MINGW%;%PATH%
```

For example, the minimum requirement (for Rtools33 or later) may be

Shell Command

```
### Under command mode, or save in a batch file.
SET R_HOME=C:\Program Files\R\R-3.4.0\
SET RTOOLS=C:\Rtools\bin\
SET MPI_HOME=C:\Program Files\Miscrosoft MPI\
SET PATH=%MPI_HOME%bin;%R_HOME%;%R_HOME%bin;%RTOOLS%;%PATH%
```

Note that gcc and others within Rtools will be detected by windows R, so the installation path of Rtools should be exactly the same as C:/Rtools.

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_0.2-3.tar.gz

R CMD INSTALL --build pbdMPI

R CMD INSTALL pbdMPI_0.2-3.zip
```

Warning: For other pbdR packages, it is possible to compile without further changes of configurations. However, only pbdMPI is tested regularly before any release.

8. FAQs

8.1. 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 MS-MPI. Currently, **pbdMPI** is built with 'HPC Pack 2012 R2 MS-MPI Redistributable Package' which is available at http://www.microsoft.com/en-us/download/. 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. Since **pbdMPI** version 0.3-0, there are two additional packages **pbdZMQ** (?) and **pbdCS** (?) which provide servers-client interaction building upon **pbdMPI** for parallel computing.

Originally, **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/.
- 7. Q: Does pbdMPI support long vector or 64-bit integer?A: See Section 4.
- 8. Q: Does pbdMPI support Amazon Web Services (AWS EC2)?

 A: See http://thirteen-01.stat.iastate.edu/snoweye/pbdr/?item=aws_ec2 for setting a cluster on AWS EC2.
- 9. Q: Does pbdMPI support multiple nodes in VirtualBox?
 A: See http://thirteen-01.stat.iastate.edu/snoweye/pbdr/?item=multiple_nodes for setting a cluster with two nodes in VirtualBox. It is extensible to multiple nodes by linked or full cloning with a few network modifications. A pure text file multiple_nodes.txt contains detail steps for the setting.
- 10. Q: A simple pbdMPI testing code hangs but simple MPI pure C code is working?
 A: If your VirtualBox has multiple adapters (for example, eth0 for NAT/host, eth1 using internal 192.168.*.* for MPI communication), then you may consider to bring down eth0 next.

Shell Command

```
sudo ip link set eth0 down
```

Further, you may also consider to consult network experts for IP and routing table configurations when multiple adapters are required. R/Rscript may not know multiple adapters nor how networking or routing table is setting up. It is just easier for MPI to use a single adapter, open all INPUT/OUTPUT/FORWARD ports, stop all firewall, etc. MPI is designed for high performance computing, so don't put too much extra stuffs to decline the performance. (Thanks for Alba Martínez-Ruiz and Cristina Montañola in Universidad Católica de la Ssma. Concepción, chil providing errors and issues.)

11. Q: (Linux/Unix/Mac) Can I install and run OpenMPI or MPICH locally without root permission?

A: Yes. You don't need **root** permission to install or run MPI applications. For general installation of MPI libraries, please see **pbdMPI/INSTALL** first. For example, you may install OpenMPI version 1.8.2 under any private user account by

R Script

```
tar zxvf openmpi-1.8.2.tar.gz
cd openmpi-1.8.2
./configure \
    --prefix=/home/user.id/work-my/local/ompi \
    CFLAGS=-fPIC
make
make install
```

The MPI library and binary will be installed at /home/user.id/work-my/local/ompi/. Then, you may add this path to system environment PATH by

R Script

```
export OMPI=/home/user.id/work-my/local/ompi
export PATH=$OMPI/bin:$PATH
```

8.2. Programming

- Q: What are pbdMPI's high level back-ends for embarrassingly parallel calculations?
 A: See man pages and examples of pbdLapply(), pbdSapply(), pbdApply(), and task.pull() for more details. Some options of those functions, such as pbd.mode, may be also useful for different data distribution in embarrassingly parallel calculations.
- 2. 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. A more efficient way, such as task pull parallelism, can be found in next Q&A.

Example 1:

SPMD R Script

```
suppressMessages(library(pbdMPI, quietly = 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

```
suppressMessages(library(pbdMPI, quietly = 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()
```

- 3. Q: Can I use unblocked send functions, such as isend()? Or, does isend() truly unblocked?
 - A: The answer is no for **pbdMPI** earlier than version 0.2-2, but it is changed since version 0.2-3. A temporary buffer list SPMD.NB.BUFFER is used to store all objects being sent by <code>isend()</code>. The buffer is created and cumulated in <code>.pbd_env</code>, but released as <code>wait()</code> is called. Although this may take some performance and space, this can avoid <code>gc()</code> and memory overwrite before actual sending is done.
- 4. Q: Can I run un-barrier task jobs, such as task pull parallelism, by using **pbdMPI**? A: Yes, it is relatively straightforward via **pbdMPI** API function task.pull() in SPMD. For example, the next is available in demo which has a user defined function FUN() run on workers, and master (rank 0) controls the task management.

Shell Command

```
mpiexec -np 4 Rscript -e "demo(task_pull,'pbdMPI',ask=F,echo=F)"
```

SPMD R Script (task_pull)

```
### Initial.
suppressMessages(library(pbdMPI, quietly = TRUE))

### Examples.
FUN <- function(jid){
    Sys.sleep(1)
    jid * 10
}

ret <- task.pull(1:10, FUN)
comm.print(ret)

if(comm.rank() == 0){
    ret.jobs <- unlist(ret)
    ret.jobs <- ret.jobs[names(ret.jobs) == "ret"]
    print(ret.jobs)
}</pre>
```

```
### Finish.
finalize()
```

5. Q: What if I want to run task push or pull by using **pbdMPI**?

A: No problem. As in the two proceeding 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 and independent jobs.

6. 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.

7. Q: Can I disable the MPI initialization of pbdMPI when I call library(pbdMPI)?

A: Yes, you can set a hidden variable .__DISABLE_MPI_INIT__ in the .GlobalEnv before calling library(pbdMPI). For example,

SPMD R Script

```
assign(".__DISABLE_MPI_INIT__", TRUE, envir = .GlobalEnv)
library(pbdMPI)
ls(all.names = TRUE)
init()
ls(all.names = TRUE)
finalize(mpi.finalize = FALSE)
```

Note that we are *NOT* supposed to kill MPI in the finalize step if MPI is initialized by external applications. But some memory allocated by **pbdMPI** has to be free, mpi.finalize = FALSE is set above.

To avoid some initialization issues of MPI, **pbdMPI** uses a different way than **Rmpi**. **pbdMPI** allows you to disable initializing communicators when loading the library, and later on you can call **init** to initialize or obtain communicators through .__MPI_APTS__ as in the next question.

8. 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.

8.3. MPI Errors

1. Q: If compilation successful, but load fails with segfault

Error Message

A: Basically, pbdMPI and all pbdR are tested and have stable configuration in GNU environment. However, other compilers are also possible such as Intel compiler. This message may come from the system of login node does not have a MPI system, MPI system is only allowed to be loaded in computing node, or MPI shared library is not loaded correctly and known to R. The solution is to use extra flag to R CMD INSTALL -no-test-load pbdMPI*.tar.gz, and use export LD_PRELOAD=... as the answer to the next question.

2. 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 export 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.

3. 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-mpi-type to specify the MPI type.
- Use --with-mpi-include and --with-mpi-libpath to specify the right version.
- 4. Q: (Mac) If installs successfully, but fails at initialization with

Error Message

```
Library not loaded: /usr/lib/libmpi.0.dylib
```

A: Please make sure the GNU compiler, R, OpenMPI, and **pbdMPI** are all built and installed under unified conditions, such as 64-bits environment. 32-bits R may not be able to load 64-bits OpenMPI nor **pbdMPI**.

5. 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.
- 6. 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.

7. Q: (Windows) If MPICH2 mpiexec fails with

Error Message

```
c:\>"C:\Program Files\MPICH2\bin\mpiexec.exe" âĹŠnp 2 Rscript C:\my_script.r launch failed: CreateProcess(Rscript C:\my_script.r) on failed, error 2 - The system cannot find the file specified.
```

A: Please try to use Rscript.exe in windows system.

8. 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.

9. Q: For MPICH2 and MPICH3 users, if installation fails with

Error Message

```
/usr/bin/ld: cannot find -lopa
collect2: error: ld returned 1 exit status
make: *** [pbdMPI.so] Error 1
ERROR: compilation failed for package 'pbdMPI'
```

A: By default, -lopa is required for some systems. However, some systems may not have it and can be disable with a configuration flag when install **pbdMPI**, such as R CMD INSTALL pbdMPI*.tar.gz -configure-args="-disable-opa".

10. Q: (MacOS 10.9.4 + OpenMPI 1.1.8) If compilation successful, but test load fails with MCA errors such as "Symol not found"

Error Message

A: The potential problem here is that mpicc -showme provides extra information, such as multiple include and library paths, and configure is not able to parse correctly. Therefore, it is easier to manually specify correct paths via -configure-args to R. (Thanks for Eilidh Troup in University of Edinburgh, Scotland providing errors and solutions.)

R Script

```
$ mpicc --showme:compile
-I/usr/local/Cellar/open-mpi/1.8.1/include
$ mpicc --showme:link
-L/usr/local/opt/libevent/lib
    -L/usr/local/Cellar/open-mpi/1.8.1/lib -lmpi

$ R CMD INSTALL pbdMPI_0.2-4.tar.gz \
    --configure-args="--with-mpi-type=OPENMPI \
    --with-mpi-include=/usr/local/Cellar/open-mpi/1.8.1/include \
    --with-mpi-libpath=/usr/local/Cellar/open-mpi/1.8.1/lib"
```

Note that ACX_MPI is also a good solution to fix configure.ac, however, it may screw up other platforms, such as Solaris, and upset CRAN. Anyone is welcome to submit a thoughful solution.

11. Q: (Windows) If OpenMPI mpiexec fails with

Error Message

```
d:/Compiler/gcc-4.9.3/mingw_32/bin/gcc
-I"D:/RCompile/recent/R-3.3.1/include" -DNDEBUG
-I"C:/Program Files/Microsoft MPI/Inc/" -DMPI2 -DWIN
-DMSMPI_NO_DEPRECATE_20
-I"d:/Compiler/gcc-4.9.3/local330/include"
-03 -Wall -std=gnu99 -mtune=core2 -c comm_errors.c -o comm_errors.o
```

A: The C:/Program Files/Microsoft MPI/Inc/ may not exist for the MS-MPI v7.1 SDKs. The header file may in a different installation directory at C:/Program Files (x86)/Microsoft SDKS/MPI/. See Section 7 for details.

8.4. Other Errors

1. Q: pbdMPI is linked with pbdPROF (?) and mpiP (?). (i.e. --enable-pbdPROF is used in pbdMPI and --with-mpiP is used in pbdPROF.) If pbdMPI compilation successful, but load fails with

Error Message

```
Error : .onLoad failed in loadNamespace() for 'pbdMPI', details:
   call: dyn.load(file, DLLpath = DLLpath, ...)
   error: unable to load shared object 'pbdMPI.so':
   pbdMPI/libs/pbdMPI.so: undefined symbol: _Ux86_64_getcontext
```

A: Some prerequisite packages by mpiP is installed incorrectly. Reinstall mpiP by

R Script

```
./configure --disable-libunwind CPPFLAGS="-fPIC
-I/usr/lib/openmpi/include" LDFLAGS="-L/usr/lib/openmpi/lib
-lmpi"
```

and followed by reinstall **pbdPROF** and **pbdMPI**.