Guide to the **pbdPROF** Package

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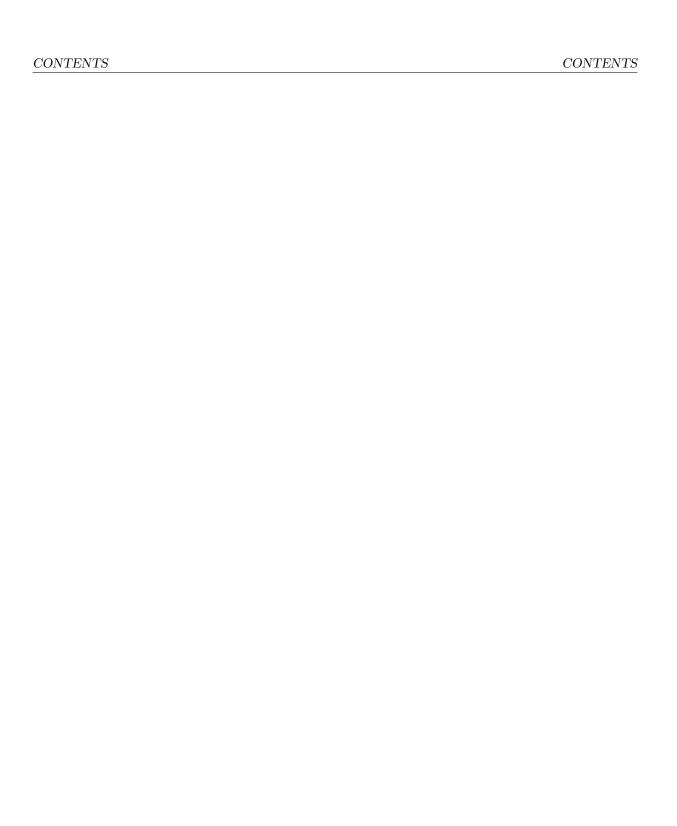Oak Ridge, TN, USA

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This document is written to explain the main functions of **pbdPROF** (Sehrawat *et al.*, 2013), version 0.1-0. 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

The goal of **pbdPROF** is to utilize external MPI profiling libraries, such as **fpmpi** (Gropp, 2000), **mpiP** (Vetter and McCracken, 2001), or **TAU** (Shende and Malony, 2006), to profile parallel R code and understand hidden MPI communications between processors. Numbers of communications, sizes of messages, times and types of functions calls all affect program performance and design of algorithm. The MPI profiling libraries are able to high-jack MPI functions at run time that intercept some of MPI function calls, then provide MPI information without disturbing original programs or algorithms.

The current main features of **pbdPROF** include:

1. providing linking information to pbdR (Ostrouchov *et al.*, 2012),

2. output profiling information associated with MPI calls,

3. parsing and summarizing profiling information, and

4. support three MPI profiling libraries.

1.1   System Requirements

pbdPROF requires an MPI installation, such as OpenMPI or MPICH2, and it also profiles an MPI-using package, such as **pbdMPI** (Chen *et al.*, 2012a) or **Rmpi** (Yu, 2002). For information regarding how to install MPI or **pbdMPI**, please see the **pbdMPI** vignette (Chen *et al.*, 2012b) or the pbdR website http://r-pbd.org/.

2   Installation

The **pbdPROF** currently is by default using **fpmpi** library internally, i.e., a source copy of **fpmpi** is located at **pbdPROF/src/fpmpi** and built in a static library at **pbdPROF/lib/libfpmpi.a**. However, external profiling libraries such as **fpmpi**, **mpiP**, and **TAU** can be also linked by **pbdPROF** via suitable `--configure-args` to R CMD INSTALL. We explain the whole procedure in Section 2.1 using **fpmpi** as an example and leave some keys steps for **mpiP** and **TAU** in furture Sections.

No matter using **fpmpi**, **mpiP**, or **TAU**, we strongly recommend to add `CPPFLAGS="-fPIC"` at the `configure` step.

2.1 fpmpi

Using internal **fpmpi** library, via

<div align="center">Shell Command</div>

```
R CMD INSTALL pbdPROF_0.1-0.tar.gz
```

By default, this compiles `src/fpmpi/*`, generates a static library `libfpmpi.a`, and installs the library to `pbdPROF/lib/`. No shared library is generated or needed, so the directory `pbdPROF/libs/` is empty (no need to build `pbdPROF.so`.) The linking argument is saved in `Makeconf` and installed to `pbdPROF/etc/` for further linking such as **pbdMPI** is reinstalled with `--enable-pbdPROF`.

Linking with external **fpmpi** library, via

<div align="center">Shell Command</div>

```
R CMD INSTALL pbdPROF_0.1-0.tar.gz \
   --configure-args="--with-fpmpi='/path_to_fpmpi/lib/libfpmpi.a'"
```

or

<div align="center">Shell Command</div>

```
R CMD INSTALL pbdPROF_0.1-0.tar.gz \
   --configure-args="--with-fpmpi='-L/path_to_fpmpi/lib -lfpmpi'"
```

Since **fpmpi** only builds a static library `libfpmpi.a`, there is no difference of these two installations of **pbdPROF**. This only provides the linking arguments either `/path_to_fpmpi/lib/libfpmpi.a` or `-L/path_to_fpmpi/lib -lfpmpi` which is saved in `Makeconf` and installed to `pbdPROF/etc/` for further linking such as **pbdMPI** is reinstalled with `--enable-pbdPROF`.

2.1.1 Reinstall pbdMPI

Reinstall **pbdMPI** via

<div align="center">Shell Command</div>

```
R CMD INSTALL pbdMPI_1.0-0.tar.gz --configure-args="--enable-pbdPROF"
```

Note that the `pbdMPI/R/get_conf.r` and `pbdMPI/R/get_lib.r` are used in `pbdMPI/configure.ac` or `pbdMPI/configure` to determine an appropriate linking flag `PROF_LDFLAGS` based on preset flags in `pbdPROF/etc/Makeconf`.

If the internal library is used in **pbdPROF**, then the path to the `pbdPROF/lib/libfpmpi.a` is set in the flag `PKG_LIBS` of `pbdMPI/src/Makevars.in`. If the external library is used in **pbdPROF**, then the linking arguments either `/path_to_fpmpi/lib/libfpmpi.a` or `-L/path_to_fpmpi/lib -lfpmpi` is set in the flag `PKG_LIBS` of `pbdMPI/src/Makevars.in`. Therefore, the **pbdMPI** can be intercepted by the **fpmpi** library when MPI function calls are evoked.

No mater the external or internal library is used, the `PROF_LDFLAGS` in `pbdMPI/etc/Makefile` provides the linking information to the profiling library. It is also used in `PKG_LIBS` which will be export to other **pbdR** packages at installation via the flag `SPMD_LDFLAGS`, therefore, no need to add further flags to `R CMD INSTALL` when reinstall packages for further profiling.

2.1.2   Reinstall pbdBASE

For further profiling, such as **pbdBASE** (Schmidt *et al.*, 2012), one may reinstall the package, via

<div align="center">Shell Command</div>

```
R CMD INSTALL pbdBASE_0.2-2.tar.gz
```

There is no need to provide any flag since **pbdMPI/etc/Makefile** has the information and installation of **pbdBASE** already considers it. Note that since both packages (**pbdMPI** and **pbdBASE**) have MPI C functions involved, it is necessary to link with profiling library in order to profile communications evoked by the package.

2.1.3   Reinstall Rmpi

Reinstall **Rmpi** via

<div align="center">Shell Command</div>

```
wget https://github.com/snoweye/Rmpi_PROF/archive/master.zip
unzip master.zip
mv Rmpi_PROF-master Rmpi
find ./Rmpi -type f -perm 777 -print -exec chmod 644 {} \;
find ./Rmpi -type d -perm 777 -print -exec chmod 755 {} \;
chmod 755 ./Rmpi/configure
chmod 755 ./Rmpi/cleanup
chmod 755 ./Rmpi/inst/*.sh
R CMD build --no-resave-data Rmpi
R CMD INSTALL Rmpi_0.6-4.tar.gz --configure-args="--enable-pbdPROF'"
```

Note that 0.6-4 is not an official release of **Rmpi**. It is a modified version of 0.6-3 and it is currently available at https://github.com/snoweye/Rmpi_PROF. The authors of **Rmpi** have plans to eventually incorporate these changes, once a stable version of **pbdPROF** hits the CRAN.

3   Test Scripts

We provide two short R scripts for **pbdMPI** and **Rmpi** to test the installation of profiling libraries and **pbdPROF**. If installation is correct, one may profile the following scripts to obtain correcponding outputs.

3.1   Test with pbdMPI

Below we provide sample scripts to test that the installation of **pbdPROF** was successful. For **pbdMPI**, use:

<div align="center">Test script for pbdMPI</div>

```
### Save this in a file: prof_pbdMPI.r
library(pbdMPI, quiet = TRUE)
init()

set.seed(comm.rank())
```

```
x <- allreduce(rnorm(100), op = "sum")

finalize()
```

and run this code by

R Script

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

A successful output of **fpmpi** in the profiling file `fpmpi_profile.txt` may contain

```
Details for each MPI routine
                 Average of sums over all processes
                                            % by message length
                              (max over        0.........1.........1........
                               processes [rank])      K         M
MPI_Allreduce:
        Calls     :              2             2 [    0] 05000000050000000000000000000
        Time      :     3.61e-05      3.72e-05 [    0] 07000000030000000000000000000
        Data Sent :           804           804 [    0]
        SyncTime  :       0.00149       0.00287 [    0] 0*0000000.000000000000000000
        By bin    : 1-4 [1,1]     [    2.5e-05,   2.72e-05] [   4.1e-05,    0.00286]
                  : 513-1024    [1,1]    [      1e-05,      1e-05] [   1.1e-05,
                      7.61e-05]
```

In this R script, one MPI C function `MPI_Allreduce` is called twice and 804 bytes are sent that a hundred of double precision (8 bytes) for 100 normal random variables, and one integer (4 bytes) for checking data type to call the corresponding S4 method.

3.2   Test with **Rmpi**

For **Rmpi**, use:

Test script for pbdMPI

```
### Save this in a file: prof_Rmpi.r
library(Rmpi, quiet = TRUE)
mpi.comm.dup(0, 1)

set.seed(mpi.comm.rank())
x <- mpi.allreduce(rnorm(100), type = 2, op = "sum")

mpi.quit()
```

and run this code by

R Script

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

A successful output of **fpmpi** in the profiling file `fpmpi_profile.txt` could be

```
Details for each MPI routine
                Average of sums over all processes
                                             % by message length
                              (max over         0.........1........1........
                              processes [rank])       K         M
MPI_Allreduce:
       Calls     :           1            1 [   0] 000000000*000000000000000000
       Time      :    4.01e-05     4.41e-05 [   1] 000000000*000000000000000000
       Data Sent :         800          800 [   0]
       SyncTime  :     0.00103      0.00204 [   1] 000000000*000000000000000000
       By bin    : 513-1024     [1,1]    [   3.6e-05,  4.41e-05] [ 2.79e-05,   0
.00204]
MPI_Comm_dup:
       Calls     :           1
       Time      :    5.81e-05
       SyncTime  :    0.000211
```

Two MPI `C` functions `MPI_Allreduce` and `MPI_Comm_dup` are called one time for each.

4   Profiling with fpmpi

4.1   Demo of pbdMPI

The `allreduce.r` is originally in **pbdMPI/demo/** and can be profiled by

R Script

```
mpiexec -np 2 Rscript -e "demo(allreduce,'pbdMPI',ask=F,echo=F)"
```

which will provide an output file `fpmpi_profile.txt`. Part of output is listed in the next as

```
Processes:        2
Execute time:   1.176
Timing Stats: [seconds] [min/max]        [min rank/max rank]
  wall-clock: 1.176 sec 1.171488 / 1.180277      0 / 1
        user: 0.378 sec 0.360000 / 0.396000      0 / 1
         sys: 0.07 sec  0.040000 / 0.100000      1 / 0


                  Average of sums over all processes
Routine                   Calls        Time Msg Length    %Time by message length
                                                   0.........1........1........
                                                         K         M
MPI_Allreduce      :        10    0.000118         188 061003000000000000000000000
MPI_Barrier        :        21     0.0054

Details for each MPI routine
                Average of sums over all processes
                                             % by message length
                              (max over         0.........1........1........
                              processes [rank])       K         M
MPI_Allreduce:
```

```
         Calls      :            10            10 [    0] 0510040000000000000000000000000
         Time       :     0.000118      0.000119 [    0] 0610030000000000000000000000000
         Data Sent  :           188           188 [    0]
         SyncTime   :     0.000312      0.000453 [    0] 07.00200000000000000000000000000
         By bin     : 1-4 [5,5]     [  7.01e-05,  7.01e-05] [  0.000117,   0.000343]
                    : 5-8 [1,1]     [  7.87e-06,  9.06e-06] [  9.06e-06,   9.06e-06]
                    : 33-64         [4,4]   [  3.91e-05,  4.03e-05] [  4.51e-05,
                         0.0001]
MPI_Barrier:
         Calls      :            21
         Time       :        0.0054
```

Two MPI C functions `MPI_Allreduce` and `MPI_Barrier` are evoked inside this R code. The `MPI_Allreduce` is called 10 times, span 0.000156 seconds, and 188 bytes are sent. The `MPI_Barrier` is called 21 times and span 0.00608 seconds.

4.2   Demo of pbdDMAT

The `svd.r` is originally in **pbdDMA/demo/** (Schmidt *et al.*, 2012) and can be profiled by

<div align="center">R Script</div>

```
mpiexec -np 2 Rscript -e "demo(svd,'pbdDMAT',ask=F,echo=F)"
```

which will provide an output file `fpmpi_profile.txt`. Part of output is listed in the next as

```
Processes:      2
Execute time:   1.774
Timing Stats: [seconds] [min/max]        [min rank/max rank]
  wall-clock: 1.774 sec 1.766181 / 1.781962      1 / 0
        user: 0.962 sec 0.956000 / 0.968000      1 / 0
         sys: 0.046 sec 0.044000 / 0.048000      0 / 1


                  Average of sums over all processes
Routine                   Calls       Time Msg Length    %Time by message length
                                                  0.........1........1........
                                                        K         M
MPI_Allreduce       :        12    0.000108          72 064000000000000000000000000000
MPI_Barrier         :         8    0.000784

Details for each MPI routine
                  Average of sums over all processes
                                               % by message length
                                (max over      0.........1........1........
                                 processes [rank])      K         M
MPI_Allreduce:
         Calls      :            12            12 [    0] 055000000000000000000000000000
         Time       :     0.000108      0.000113 [    0] 064000000000000000000000000000
         Data Sent  :            72            72 [    0]
         SyncTime   :     0.000143       0.00016 [    1] 064000000000000000000000000000
         By bin     : 1-4 [6,6]     [  5.44e-05,  6.91e-05] [  6.91e-05,  8.89e-05]
                    : 5-8 [6,6]     [  4.36e-05,  4.79e-05] [  5.72e-05,  7.08e-05]
MPI_Barrier:
         Calls      :             8
```

```
        Time      :     0.000784
```

Two MPI C functions `MPI_Allreduce` and `MPI_Barrier` are evoked inside this R code. The `MPI_Allreduce` is called 12 times, span 0.000108 seconds, and 72 bytes are sent. The `MPI_Barrier` is called 8 times and span 0.000784 seconds.

4.3   Demo of Rmpi

The `masterSlavePI.r` is originally in **Rmpi/demo/** and can be profiled by

R Script

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

which will provide an output file `fpmpi_profile.txt`. Part of output is listed in the next as

```
Processes:      1
Execute time:   0.05362
Timing Stats: [seconds] [min/max]      [min rank/max rank]
  wall-clock: 0.05362 sec      0.053622 / 0.053622     0 / 0
        user: 0.236 sec 0.236000 / 0.236000     0 / 0
         sys: 0.052 sec 0.052000 / 0.052000     0 / 0


                  Average of sums over all processes
Routine                Calls      Time Msg Length    %Time by message length
                                              0.........1........1........
                                                       K         M
MPI_Reduce        :      1    6.51e-05      8 00*000000000000000000000000000

Details for each MPI routine
                  Average of sums over all processes
                                              % by message length
                             (max over      0.........1........1........
                              processes [rank])      K         M
MPI_Reduce:
       Calls    :          1           1 [   0] 00*000000000000000000000000000
       Time     :    6.51e-05    6.51e-05 [   0] 00*000000000000000000000000000
       Data Sent :         8           8 [   0]
       By bin   : 5-8 [1,1]   [  6.51e-05,  6.51e-05]
```

One MPI C function `MPI_Reduce` is evoked inside this R code. The `MPI_Reduce` is called only 1 time, span $6.51e - 05$ seconds, and 8 bytes are sent. Note that there is only one processor (master in `comm=0`) profiled by **fpmpi**, and the other three processors (slaves in `comm=1`) are not.

5   Debugging pbdPROF

5.1   Installation related problems

Problem:1.If you have downloaded the package from github and tried to using R CMD INSTALL **pbd-PROF** and you see an error similar to this

```
ERROR: 'configure' exists but is not executable -- see the 'R Installation and
    Administration Manual'
```

Solution:You have to make the configure executable which means giving it permission , which can done by

<div align="center">R Script</div>

```
chmod +x configure
```

after changing the folder to package's main directory.

Problem:2.If you are using **fpmpi** (Gropp, 2000) externally and during it's installation you get an error similar to this

```
error :checking for library containing MPI_Init... (cached) no configure:
error: Could not find MPI library
```

Solution: You probably need to specify the path to MPI library using this in command line in the fpmpi main directory

<div align="center">R Script</div>

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

5.2   Error on running

Problem:1.While Running **Rmpi** code for profiling and you encounter the below error:

```
error: mpiexec was unable to launch the specified application as it could not
    access
or execute an executable:
Executable: /path/to/R/package_installation_directory/2.15/Rmpi/Rslaves.sh
Node: "Your_node"
while attempting to start process rank 0.
```

Solution:You need to make executable of the shell scripts in the "inst" directory of "Rmpi" main directory using the following command from command line in "inst" directory:

<div align="center">R Script</div>

```
chmod +x *.sh
```

Problem:2.While Running **Rmpi** code for profiling and you are encountering the below error:

```
[G:12221] [[39704,0],0] ORTE_ERROR_LOG: Not found in file
    ../../../../../orte/mca/plm/base/plm_base_launch_support.c at line 758
```

```
------------------------------------------------------------------------
mpiexec was unable to start the specified application as it encountered an
    error.
More information may be available above.
------------------------------------------------------------------------
```

Solution:

1. You need to check whether your **Rmpi** is working without the **pbdPROF**.If yes try running your **Rmpi** code on single process only.

2. If above does not help, then you may need .Rprofile in Rmpi/inst/ to run your code from "inst" directory.

3. If still your code does not run ,you need to update your OPENMPI version to the latest one.You can check your openmpi version http://www.open-mpi.org/software/ompi/ through

```
ompi_info
```

4. If further you came to this far and luck is not with you somehow(pun intended), there might some configuration problem in your machine.

6 References

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