A Quick Guide for the pbdSLAP Package

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Warning: This document is written to explain the main functions of **pbdSLAP**˜(Chen *et˜al.* 2012c), 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: `http://r-pbd.org/`.

1. Quick Start

The **pbdSLAP** package serves as a mechanism to utilize a subset of functions from the ScaLAPACK˜(Blackford *et˜al.* 1997) library from within R˜(R Core Team 2012), and in particular from the higher level R packages **pbdBASE**˜(Schmidt *et˜al.* 2012a) and **pbdDMAT**˜(Schmidt *et˜al.* 2012b). It allows one to merely "plug in" the necessary libraries without needing to do a complicated system installation. It is a bundling of the official ScaLAPACK distribution from the ScaLAPACK Team at netlib (`http://www.netlib.org/scalapack/`). However, it is possible to use other ScaLAPACK libraries instead; see Section˜2.2 for details.

The **pbdSLAP** package consists of a minimum set of double precision functions from the **ScaLAPACK** library for R's distributed matrix computation. **ScaLAPACK** includes many important functions for distributed linear algebra, including LU factorization, singular value decomposition, etc. We also include the necessary components of the libraries that our subset of **ScaLAPACK** relies on, namely **BLACS**, **PBLAS**, **BLAS**, and **LAPACK**.

The system requirements and installation instructions for **pbdSLAP** are provided in the following section. A technical issue for grid information of **BLACS** is described in the Section˜4.

1.1. System Requirements

pbdSLAP requires **pbdMPI**˜(Chen *et˜al.* 2012a), which itself requires a system installation of MPI. (`http://en.wikipedia.org/wiki/Message_Passing_Interface`). **pbdSLAP** should also work with LAM/MPI (`http://www.lam-mpi.org/`) and MPICH2 (`http://www.mcs.anl.gov/research/projects/mpich2/`).

pbdSLAP is mainly developed and tested under OpenMPI (`http://www.open-mpi.org/`) in Xubuntu 11.04 and 12.04 systems (`http://xubuntu.org/`). **pbdSLAP** should also run on other operating systems, such as Mac with OpenMPI, or Windows with MPICH2 if MPI is installed and launched properly. However, we have not extensively tested installation and use of the **pbd** toolchain on other platforms. The reader is encouraged to report his/her experience with **pbdSLAP** on other platforms.

1.2. Installation and Quick Start

The remaining assumes that **pbdMPI** is installed correctly. If **pbdMPI** is not yet installed, see the **pbdMPI** vignette˜(Chen *et˜al.* 2012b) for installation details. Users can download **pbdSLAP** from CRAN at `http://cran.r-project.org`, and the installation can be done with the following commands

Shell Command

```
tar zxvf pbdSLAP_0.1-0.tar.gz
R CMD INSTALL pbdSLAP
```

Users can get started quickly with **pbdSLAP** by learning from the following example.

Shell Command

```
### Under command mode, run the demo with 2 processors by
### (Use Rscript.exe for windows system)

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

2. Useful Information

2.1. CDEFS~Flag of ScaLAPACK

The `CDEFS` is a flag for interface between C and Fortran, and is required to compile **pbdSLAP**. `CDEFS = -DAdd_` is the default for GNU C and Fortran. The correct value can be determined by BLACS test intface tool in `pbdSLAP/inst/intface/`. For other compilers, the possible values could be `-DNoChange`, `-Df77IsF2C`, or `-DUpCase`.

For other values, user can provide an external `CDEFS` flag at installation time, such as

Shell Command

```
tar zxvf pbdMPI_0.1-0.tar.gz
R CMD INSTALL pbdSLAP \
  --configure-vars="CDEFS='other possible flags'"
```

The value of `CDEFS` (other possible flags) can be one of the possible values above or other configurations. For PGI compiler, the value could be `-DAdd_ -DNO_IEEE $(USEMPI)`. Note that the `CDEFS` will overwrite the default `CDEFS` inside `pbdSLAP/src/Makevars.in` for compiling `libslap.a`.

2.2. Using Other Distributions of ScaLAPACK

Some users may have access to other, often non-free, distributions of Scalapack, such as Intel's **MKL** (http://software.intel.com/en-us/intel-mkl) or Cray's **LibSci** (http://docs.cray.com/). It may be possible to achieve some performance gains using these libraries over netlib ScaLAPACK, especially when using big machines, such as Nautilus and Kraken in NICS (http://www.nics.tennessee.edu).

To use these external libraries with **pbdSLAP**, you need only supply the appropriate flag to `EXT_LDFLAGS` at compile time. Specifically, the user would issue the command:

Shell Command

```
tar zxvf pbdMPI_0.1-0.tar.gz
R CMD INSTALL pbdSLAP \
  --configure-vars="EXT_LDFLAGS='external ldflags'"
```

where "external ldflags" needs to include linking information to ScaLAPACK, BLACS, LAPACK, and BLAS. Please be aware that the order matters in the `EXT_LDFLAGS`. Note that `EXT_LDFLAGS` will be part of `PKG_LDFLAGS` inside `pbdSLAP/src/Makevars.in`.

3. Inside pbdSLAP

Currently, **pbdSLAP** only supports MPI systems for communication. Some packages currently utilizing **pbdSLAP** are **pbdBASE** and **pbdDMAT**, which use R's S4 classes and methods for distributed matrix computations. For details, see the vignettes˜(Schmidt *et˜al.* 2012c,d) of **pbdBASE** and **pbdDMAT**. **pbdSLAP** also provides a linking mechanism to export the library `libslap.a` for other applications.

3.1. Linking with pbdSLAP

pbdSLAP provides a static library `libslap.a` which is useful to link into other applications. For furture reference, all linking information is stored in the file

`${R_HOME}/library/pbdSLAP/etc${R_ARCH}/Makeconf`

including the header files to **pbdMPI** and **pbdSLAP**, as well as the path to `libslap.a` or, if utilized, the external libraries such as **MKL**. An example configuration can be found in `pbdBASE/src/Makevars.in`. The linking flags are available from

pbdBASE/src/Makevars.in

```
R_SCMD = ${R_HOME}/bin/Rscript -e
SLAP_LDFLAGS = $(shell ${R_SCMD} \
  "source('../R/get_lib.r'); \
   get.lib('R_SLAP','"${R_ARCH}"')")
```

It is also very likely to link with **pbdMPI** since MPI is a prerequisite. One can obtain the system's MPI information from **pbdMPI**, and the linking flags are available from

pbdSLAP/src/Makevars.in

```
R_SCMD = ${R_HOME}/bin/Rscript -e
SPMD_CPPFLAGS = $(shell ${R_SCMD} \
  "source('../R/get_conf.r'); \
   get.conf('PKG_CPPFLAGS','"${R_ARCH}"')")
SPMD_LDFLAGS = $(shell ${R_SCMD} \
  "source('../R/get_conf.r'); \
   get.conf('PKG_LIBS','"${R_ARCH}"')")
```

where `$R_ARCH` is avaialbe from the default R `Makeconf` file.

4. Testing BLACS

Strictly speaking, **pbdSLAP** does not use the original way of interacting with **BLACS** to deal with grid information. In **BLACS**, the grid information is pointers pointing to C structures containing MPI communicators for grid construction. The `ICTXT` value of the C structure is the original way for Fortran to access MPI communicators.

In R, specifically **pbdBASE**, we use hidden global R objects (`.__grid_info_*`) to store the grid information, where `*` is an integer depending on the BLACS context id (`ictxt`) for the grid initialized by function (`slap.init.grid`).

When computing is finished, we need to exit all the BLACS grids. For each grid, `slap.exit.grid` function can free the grid via the id (`ictxt`). Initially, the maximum number of `ICTXT` is `10` in **BLACS**, but can be dynamically allocated if this maximum is reached. Users do not need to directly manage this.

When all grids exit completely, we need to finalize **pbdSLAP** by calling `slap.finalize`, and by default MPI is usually not finalized. `slap.finalize` will take care of freeing memory before quiting the **pbdSLAP**.

Now save the next script in a file and run with

Shell Command

```
mpirun -np 4 Rscript gridinfo.r
```

to see the grid information. This example provides four grids `ictxt = 0,1,2,3` in R, but `0, 1` are exited before initializing `2, 3`. The `ICTXT` shows that only `0, 1` in Fortran are used twice for all grids.

SPMD R Script

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

slap.init.grid(2, 2, ictxt = 0)
slap.init.grid(1, 4, ictxt = 1)

comm.cat(">> .__grid_info_0\n", quiet = TRUE)
comm.print(.__grid_info_0, all.rank = TRUE)
comm.cat(">> .__grid_info_1\n", quiet = TRUE)
comm.print(.__grid_info_1, all.rank = TRUE)

slap.exit.grid(0)
slap.exit.grid(1)

slap.init.grid(4, 1, ictxt = 2)
slap.init.grid(2, 3, ictxt = 3)

comm.cat(">> .__grid_info_2\n", quiet = TRUE)
comm.print(.__grid_info_2, all.rank = TRUE)
comm.cat(">> .__grid_info_3\n", quiet = TRUE)
comm.print(.__grid_info_3, all.rank = TRUE)

slap.exit.grid(2)
slap.exit.grid(3)

slap.finalize()
finalize()
```

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