

A Quick Guide for the pbdBASE Package

Version 2.0

Drew Schmidt¹, Wei-Chen Chen², George Ostrouchov^{1,2},
Pragneshkumar Patel¹

¹Remote Data Analysis and Visualization Center
University of Tennessee,
Knoxville, TN, USA

²Computer Science and Mathematics Division,
Oak Ridge National Laboratory,
Oak Ridge, TN, USA

Contents

Acknowledgement	ii
Abstract	1
1. Introduction	1
1.1. Installation	1
1.2. Indented Audience	1
1.3. Terminology	2
2. Using pbdBASE	2
2.1. BLACS Communicators	2
2.2. Advanced Users	3
References	4

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Abstract

With the size of data ever growing, the use of multiple processors in a single analysis becomes more and more a necessity. The Programming Big Data in R (pbdR) project attempts to address the R language's current shortcomings in parallel distributed computations. The **pbdBASE** package for R provides a set of BLACS, PBLAS, and ScaLAPACK wrappers, as well as numerous new functionality in the block-cyclic matrix paradigm. In addition to performance improvements through parallelism, use of this system with more than one processor allows the user to break R's local memory barrier, namely the requirement that a vector be indexed by a 32-bit integer, by only storing subsets of the vector on each processor.

1. Introduction

The Programming with Big Data in R (Ostrouchov *et al.* 2012), abbreviated pbdR or just pbd, is a project which seeks to elevate the R language to supercomputers. This package, **pbdBASE** (Schmidt *et al.* 2012a), contains a set of wrappers of the high performance libraries BLACS, PBLAS, and ScaLAPACK (Blackford *et al.* 1997), and also a host of new subroutines for performing distributed matrix computations in R. The package is a dependency of **pbdDMAT** (Schmidt *et al.* 2012b), which is meant to greatly simplify the **pbdBASE** system into something that intimately resembles the R language. Since these two packages ultimately rely on the ScaLAPACK library, the data type used with each is the block-cyclic distributed matrix. See the **pbdDMAT** vignette for more details.

Updates and bug releases for this and other **pbd** projects may, especially while in infancy, be much more frequent than CRAN releases. So for up to date packages, as well as evolving information about the **pbd** project, see the pbdR project's github <http://code.r-pbd.org> or our website <http://r-pbd.org/>.

1.1. Installation

The **pbdBASE** package is available from the CRAN at <http://cran.r-project.org>, and can be installed via a simple

Installing pbdBASE

```
install.packages("pbdBASE")
```

This assumes only that you have MPI installed and properly configured on your system. If the user can successfully install the package's two principal dependencies, **pbdMPI** (Chen *et al.* 2012a) and **pbdSLAP** (Chen *et al.* 2012c) (each available from the CRAN), then the installation for **pbdBASE** should go smoothly. If you experience difficulty installing either these packages, you should see their documentation.

1.2. Intended Audience

The **pbdBASE** package is a dependency of **pbdDMAT**, and so anyone who wishes to use the latter package must first install **pbdBASE**. However, much of the direct use of **pbdBASE** is intended only for extremely advanced users and developers. A few exceptions are the

`init.grid()` and `finalize()` functions, which will be outlined in the sections to follow. The overwhelming majority of the remaining functions are either internal or for people deeply familiar with ScaLAPACK.

1.3. Terminology

Before beginning, we will make frequent use of concepts from the Single Program/Multiple Data (SPMD) paradigm. If you are entirely unfamiliar with this approach to parallelism, or if you are unfamiliar with the **pbdMPI** package, then you are strongly encouraged to read the vignette (Chen *et al.* 2012b) contained in the **pbdMPI** package, as well as examine and digest its many examples in order to better understand what follows.

A concise explanation of SPMD is that it is an approach to parallel, distributed programming in which one program is written, and each processor runs that same program, though that program locally will often be interacting with different data. This, in contrast to the manager/worker paradigm where one processor, the manager, is in charge of its workers, each of whom swear fealty to the manager. So in SPMD, each processor believes itself to be the manager, the one in charge. As a colleague, Dr. Russell Zaretzki put it, “it’s like academia.”

2. Using pbdBASE

2.1. BLACS Communicators

Briefly, distributed matrix computations using ScaLAPACK require specialized MPI communicators, via the BLACS library. As with any MPI communicator, you must initialize it before getting started with communications, and you must terminate it when you are finished with communications. For most users, this will amount to calling

```
library(pbdBASE, quiet = TRUE)
init.grid() # initialize

# ...

finalize() # terminate
```

This special communicator may be used with **pbdMPI** communicator(s) without causing problems, and by default one `finalize()` call will terminate all communicators, whether they be from **pbdMPI** or **pbdBASE** (see the **pbdBASE** reference manual for more details and options).

However, BLACS communicators are not identical to **pbdMPI** communicators. Indeed, while a **pbdMPI** communicator is a one-dimensional array of processors, BLACS communicators are two-dimensional (row-major) grids. These values are simply referred to as the number of processor rows and the number of processor columns, as a communicator really is thought of as a matrix of processors. When a grid is initialized with `init.grid()` and no arguments are passed, then three communicators are created. These grids are referenced by their “integer

context” value, or `ICTXT`. These grids are numbered 0, 1, and 2. Context 0 tries to be the “best possible” context (see (Blackford *et al.* 1997)). Here we make 2 choices:

1. Grids are always as close to square as possible.
2. In the event a grid can not be made to be square, the larger value is used for the number of processor rows.

So for example, if we have 4 processors, then by default this would create a 2×2 grid for context 0. However, if we have 6 processors, then by default this will create a 3×2 grid of processors.

On the other hand, context 1 is always a $1 \times n$ grid, where n is the total number of processors. Likewise, context 2 is always a $n \times 1$ grid of processors. These can be extremely valuable, especially for performing data movement operations.

2.2. Advanced Users

This section assumes that you are familiar with the various paradigms of the BLACS, PBLAS, and ScaLAPACK libraries.

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