# Programming with Big Data in R

Drew Schmidt and George Ostrouchov

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# Affiliations and Support

The pbdR Core Team <a href="http://r-pbd.org">http://r-pbd.org</a>

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## About This Presentation

#### **Downloads**

This presentation and supplemental materials are available at:

http://r-pbd.org/user2013



## About This Presentation

# Speaking Serial R with a Parallel Accent

The content of this presentation is based in part on the **pbdDEMO** vignette *Speaking Serial R with a Parallel Accent* 

https://github.com/wrathematics/pbdDEMO/blob/master/inst/doc/pbdDEMO-guide.pdf?raw=true

It contains more examples, and sometimes added detail.



## About This Presentation

#### Installation Instructions

Installation instructions for setting up a pbdR environment are available:

This includes instructions for installing R, MPI, and pbdR.



# About This Presentation

## Conventions

## We use:

- "•" as a decimal mark
- "," as order of magnitude separator

Example	Yes	No	
One million	1,000,000	1.000.000	
One half	0.5	0,5	
One thousand and one half	1,000.5	1.000, 5	



# Contents

- Introduction
- 2 pbdR
- 3 Introduction to pbdMPI
- 4 The Generalized Block Distribution
- Brief Intermission
- 6 Basic Statistics Examples
- Introduction to pbdDMAT
- 8 Examples Using pbdDMAT
- Wrapup



## Contents

- Introduction
  - A Concise Introduction to Parallelism
  - Common Terminology
  - R and Parallelism



A Concise Introduction to Parallelism

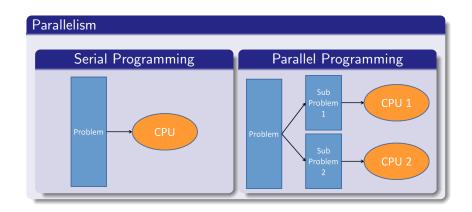
### What is Parallelism?

Broadly, doing more than one thing at a time.

The simultaneous use of multiple compute resources to solve a computational problem:

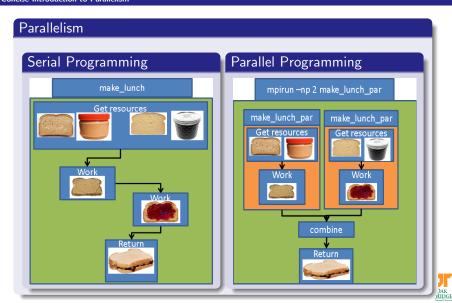


A Concise Introduction to Parallelism





A Concise Introduction to Parallelism



A Concise Introduction to Parallelism

## Kinds of Parallelism

- Data Parallelism: Data is distributed
- Task Parallelism: Tasks are distributed



A Concise Introduction to Parallelism

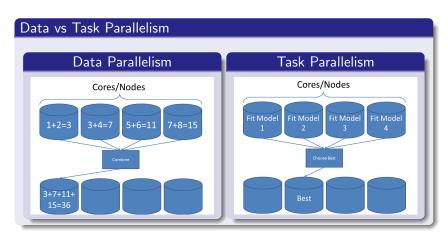
## pbdR Paradigms: Data Parallelism

With data parallelism:

- No one processor/node owns all the data.
- Processors own local pieces of a (conceptually) global object



A Concise Introduction to Parallelism





Common Terminology

## Difficulty

- Implicit parallelism: Parallel details hidden from user
- 2 Explicit parallelism: Some assembly required...
- 3 Embarrassingly Parallel: Also called loosely coupled. Obvious how to make parallel; lots of independence in computations.
- **1** Tightly Coupled: Opposite of embarrassingly parallel; lots of dependence in computations.



Common Terminology

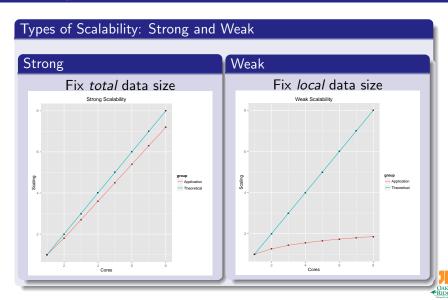
## Scalability

Scalability: unitless measure of performance;

$$\frac{\tau_i}{\tau_0}$$



Common Terminology

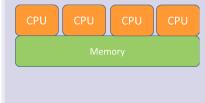


Common Terminology

## Shared and Distributed Memory Machines

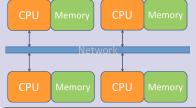
## Shared Memory

Different processors can directly access and modify each others' memory. There is only one node.



## Distributed

Different processors/nodes can not directly access/modify different processors'/nodes' memory.





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Common Terminology

# Shared and Distributed Memory Machines

# Shared Memory Machines

Thousands of cores



Nautilus, University of Tennessee

1024 cores

# Distributed Memory Machines

Hundreds of thousands of cores



112,896 cores



R and Parallelism

## R and Parallelism

What about R?



R and Parallelism

## Problems with Serial R

- Slow.
- ② If you don't know what you're doing, it's really slow.
- Open Performance improvements usually for small machines.
- 4 Very ram intensive.
- 6 Chokes on big data.



R and Parallelism

# Shared Memory 1 foreach 2 parallel 3 snow 4 multicore Distributed 1 Rmpi 2 R+Hadoop 3 pbdR



R and Parallelism

#### R and Parallelism

The solution to many of R's problems is parallelism. However . . .

## What we have

- Mostly serial.
- 2 Mostly not distributed
- Data parallelism mostly explicit

#### What we want

- Mostly parallel.
- Mostly distributed.
- Mostly implicit.



R and Parallelism

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## Why We Need Parallelism

- Saves time (long term).
- ② Data size is skyrocketing.
- 3 Necessary for many problems.
- Like it or not, it's coming.
- 1t's really cool.



## **Contents**

- 2 pbdR
  - The pbdR Project
  - pbdR Paradigms



The pbdR Project

# Programming with Big Data in R (pbdR)

Striving for Productivity, Portability, Performance



- Free<sup>a</sup> R packages.
- Bridging high-performance C with high-productivity of R
- Scalable, big data analytics.
- Distributed data details implicitly managed.
- Methods have syntax identical to R.
- Powered by state of the art numerical libraries (MPI, ScaLAPACK, . . . )



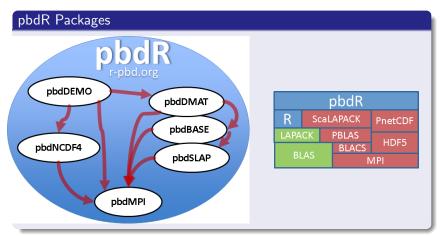
<sup>&</sup>lt;sup>a</sup>MPL, BSD, and GPL licensed

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The pbdR Project







The pbdR Project

## pbdR Packages — http://code.r-pbd.org

### Released to CRAN:

- pbdMPI: MPI bindings (explicit, low-level)
- pbdSLAP: Foreign library (just install it, nothing to use)
- pbdBASE: Compiled code (used by DMAT, also for devs)
- pbdDMAT: Distributed matrices (mostly implicit, high-level)
- pbdNCDF4: Parallel NetCDF4 reader
- pbdDEMO: Package demonstrations, examples, vignette written in textbook style

## Future Development:

- Updates and expansions
- Profiling Tools for Parallel Computing with R

. .



The pbdR Project

## Example Syntax

```
1 x <- x[-1, 2:5]

2 x <- log(abs(x) + 1)

3 xtx <- t(x) %*% x

4 ans <- svd(solve(xtx))
```

Look familiar?

The above runs on 1 core with R or 10,000 cores with pbdR



pbdR Paradigms

## pbdR Paradigms

Programs that use pbdR are utilize:

- Batch execution
- Single Program/Multiple Data (SPMD) style

And generally utilize:

Data Parallelism



pbdR Paradigms

## **Batch Execution**

- Non-interactive
- Use

```
1 Rscript my_script.r
```

or

```
1 R CMD BATCH my_script.r
```

• In parallel:

```
1 mpirun -np 2 Rscript my_par_script.r
```



# Single Program/Multiple Data (SPMD)

- SPMD is a programming *paradigm*.
- Not to be confused with SIMD.
- SPMD utilizes MIMD architecture computers.
- Arguably the simplest extension of serial programming.
- Difficult to describe, easy to do...
- Only one program is written, executed in batch on all processors.
- Different processors are autonomous; there is no manager.
- The dominant programming model for large machines.



pbdR Paradigms

SPMD			
Manager/Worker	SPMD		



## **Contents**

- 3 Introduction to pbdMPI
  - Managing a Communicator
  - Reduce, Gather, Broadcast, and Barrier
  - Other pbdMPI Tools



Managing a Communicator

## Message Passing Interface (MPI)

- MPI: Standard for managing communications (data and instructions) between different nodes/computers.
- Implementations: OpenMPI, MPICH2, Cray MPT, . . .
- Enables parallelism (via communication) on distributed machines.
- Communicator: manages communications between processors.



# MPI Operations (1 of 2)

 Managing a Communicator: Create and destroy communicators.

```
init() — initialize communicator
finalize() — shut down communicator(s)
```

 Rank query: determine the processor's position in the communicator.

```
comm.rank() — "who am I?"
comm.size() — "how many of us are there?"
```

• **Printing**: Printing output from various ranks.

```
comm.print(x)
comm.cat(x)
```

**WARNING**: only use these functions on *results*, never on yet-to-be-computed things.



Managing a Communicator

# Quick Example 1

## Rank Query: 1\_rank.r

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

my.rank <- comm.rank()
comm.print(my.rank, all.rank=TRUE)

finalize()</pre>
```

## Execute this script via:

## Sample Output:



Managing a Communicator

# Quick Example 2

## Hello World: 2\_hello.r

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

comm.print("Hello, world")

comm.print("Hello again", all.rank=TRUE, quiet=TRUE)

finalize()
```

## Execute this script via:

## Sample Output:

```
mpirun -np 2 Rscript 2_hello.r

1 COMM.RANK = 0
2 [1] "Hello, world"
3 [1] "Hello again"
4 [1] "Hello again"
```



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Reduce, Gather, Broadcast, and Barrier

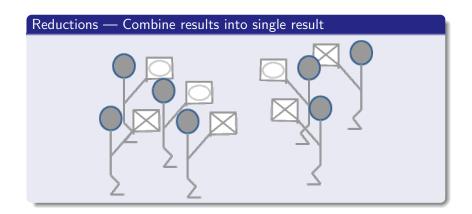
# MPI Operations

- Reduce
- Gather
- Broadcast
- Barrier



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Reduce, Gather, Broadcast, and Barrier



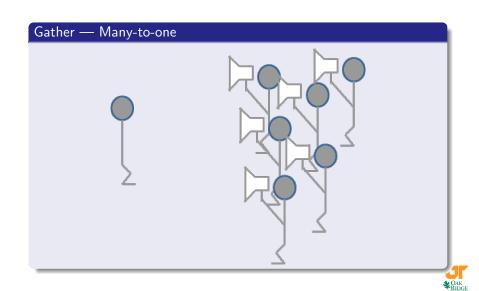


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Reduce, Gather, Broadcast, and Barrier

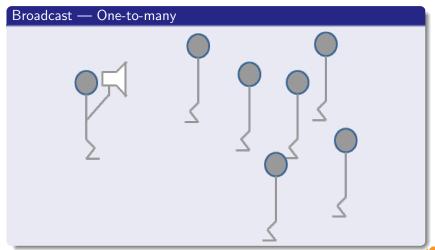




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Reduce, Gather, Broadcast, and Barrier





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# Barrier — Synchronization Barrier **Barrier** Barrier DAK UDGE

## MPI Operations (2 of 2)

- Reduction: each processor has a number x; add all of them up, find the largest/smallest, ....
   reduce(x, op='sum') reduce to one allreduce(x, op='sum') reduce to all
- Gather: each processor has a number; create a new object on some processor containing all of those numbers.
   gather(x) — gather to one allgather(x) — gather to all
- Broadcast: one processor has a number x that every other processor should also have.
   bcast(x)
- Barrier: "computation wall"; no processor can proceed until all processors can proceed.
   barrier()



## Quick Example 3

```
Reduce and Gather: 3_gt.r
```

```
library(pbdMPI, quiet = TRUE)
  init()
  comm.set.seed(diff=TRUE)
  n <- sample(1:10, size=1)
  gt <- gather(n)
  comm.print(unlist(gt))
10
  sm <- allreduce(n, op='sum')</pre>
  comm.print(sm, all.rank=T)
13
  finalize()
```

#### Execute this script via:

## Sample Output:

```
COMM.RANK = O
mpirun -np 2 Rscript 3 gt.r
                                   2 [1] 2 8
                                     COMM.RANK = O
                                   4 [1] 10
                                     COMM.RANK = 1
                                   6 [1] 10
```



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## Quick Example 4

### Broadcast: 4\_bcast.r

```
library(pbdMPI, quiet=T)
  init()
3
  if (comm.rank() == 0) {
    x <- matrix(1:4, nrow=2)
  } else {
    x <- NULL
8
  }
9
10
  v <- bcast(x, rank.source=0)</pre>
11
  comm.print(y, rank=1)
13
  finalize()
```

#### Execute this script via:

```
mpirun -np 2 Rscript 4_bcast.r
```

#### Sample Output:

```
COMM.RANK = 1
[,1] [,2]
[1,] 1 3
[2,] 2 4
```



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Other pbdMPI Tools

## MPI Package Controls

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The .SPMD.CT object allows for setting different package options with **pbdMPI**. See the entry *SPMD Control* of the **pbdMPI** manual for information about the .SPMD.CT object:

http://cran.r-project.org/web/packages/pbdMPI/pbdMPI.pdf



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## Quick Example 5

```
Barrier: 5_barrier.r
```

```
library(pbdMPI, quiet = TRUE)
  init()
  .SPMD.CT$msg.barrier <- TRUE
  .SPMD.CT$print.quiet <- TRUE
  for (rank in 1:comm.size()-1){
    if (comm.rank() == rank){
      cat(paste("Hello", rank+1, "of", comm.size(), "\n"))
10
    barrier()
11
12
13
  comm.cat("\n")
15
  comm.cat(paste("Hello", comm.rank()+1, "of",
      comm.size(), "\n"), all.rank=TRUE)
17
  finalize()
```

#### Execute this script via:

#### Sample Output:

```
mpirun -np 2 Rscript 5_barrier.r 1 Hello 1 of 2 Hello 2 of 2
```



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## Random Seeds

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**pbdMPI** offers a simple interface for managing random seeds:

- comm.set.seed(diff=TRUE) Independent streams via the rlecuyer package.
- comm.set.seed(seed=1234, diff=FALSE) All processors use the same seed seed=1234
- comm.set.seed(diff=FALSE) All processors use the same seed, determined by processor 0 (using the system clock and PID of processor 0).



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#### Quick Example 6

```
Timing: 6_timer.r
   library(pbdMPI, quiet=TRUE)
  init()
  comm.set.seed(diff=T)
   test <- function(timed)
7
    ltime <- system.time(timed)[3]</pre>
8
9
10
    mintime <- allreduce(ltime, op='min')
    maxtime <- allreduce(ltime, op='max')
11
    meantime <- allreduce(ltime, op='sum')/comm.size()
12
13
14
     return (data.frame (min=mintime, mean=meantime,
         max=maxtime))
15
16
  times <- test(rnorm(1e6)) # ~7.6MiB of data
  comm.print(times)
19
  finalize()
```

#### Execute this script via:

```
mpirun -np 2 Rscript 6_timer.r
```

#### Sample Output:

```
min mean max
2 1 0.17 0.173 0.176
```



## Other Helper Tools

000000

**pbdMPI** Also contains useful tools for Manager/Worker and task parallelism codes:

- Task Subsetting: Distributing a list of jobs/tasks get.jid(n)
- \*ply: Functions in the \*ply family.
  pbdApply(X, MARGIN, FUN, ...) analogue of apply()
  pbdLapply(X, FUN, ...) analogue of lapply()
  pbdSapply(X, FUN, ...) analogue of sapply()



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# Quick Comments for Using pbdMPI

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Start by loading the package:

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

2 Always initialize before starting and finalize when finished:

```
init()

;

;

;

;

;

finalize()
```



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Introduction pbdR pbdMPI **GBD** Break Stats eg's pbdDMAT pbdDMAT eg's Wrapup

# Contents

- The Generalized Block Distribution
  - The GBD Data Structure
  - GBD: Example 1
  - GBD: Example 2

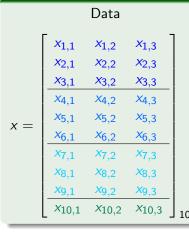


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The GBD Data Structure

# Distributing a Matrix Across 4 Processors: Block Distribution



## **Processors**



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The GBD Data Structure

# Distributing a Matrix Across 4 Processors: Local Load Balance

#### Data $x_{1,1}$ $x_{1,2}$ $x_{1,3}$ $X_{2,2}$ $x_{2,3}$ X3.1 X3,2 X3,3 X4.3 X4.1X4.2 $X_{5.1}$ X5.2 X5.3 $x_{6,2}$ $X_{6,3}$ $X_{7,3}$ X7.2 X8.1 X8.2 X8.3 X9,1 X9,2 X9,3 $X_{10,1}$ $X_{10,2}$ X<sub>10,3</sub> 10×3

## **Processors**



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The GBD Data Structure

#### The GBD Data Structure

Throughout the examples, we will make use of the Generalized Block Distribution, or GBD distributed matrix structure.

- GBD is distributed. No processor owns all the data.
- ② GBD is non-overlapping. Rows uniquely assigned to processors.
- 3 GBD is row-contiguous. If a processor owns one element of a row, it owns the entire row.
- 4 GBD is globally row-major, locally column-major.
- GBD is often locally balanced, where each processor owns (almost) the same amount of data. But this is not required.

	×8,1	<i>x</i> 8,2	<i>x</i> 8,3	
	X9,1	X9,2	X9,3	
	×10,1	<i>X</i> <sub>10,2</sub>	<i>X</i> <sub>10,3</sub>	
is adjacent (by global row) to or (by communicator number)				

X1.2

 $X_{2,2}$ 

X3.2

X4.2

X5.2

 $x_{6,2}$ 

X7.2

 $x_{1.3}$ 

 $X_{2.3}$ 

X3,3

X4.3

X5,3

 $x_{6.3}$ 

X7.3

 $x_{1.1}$ 

 $X_{2.1}$ 

X3.1

X4.1

X5.1

 $x_{6.1}$ 

 $x_{7,1}$ 

- The last row of the local storage of a processor is adjacent (by global row) to the first row of the local storage of next processor (by communicator number) that owns data.
- GBD is (relatively) easy to understand, but can lead to bottlenecks if you have many more columns than rows.



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GBD: Example 1

# Understanding GBD: Global Matrix

Processors = 0 1 2 3 4 5



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GBD: Example 1

# Understanding GBD: Load Balanced GBD

$$X = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}$$

 $Processors = 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5$ 



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GBD: Example 1

# Understanding GBD: Local View

```
X<sub>12</sub>
                 X13
                        X14
                                X<sub>15</sub>
                                        X16
                                               X17
                                                       X<sub>18</sub>
                                                               X19
 x_{21}
         X22
                 X23
                        X24
                                X25
                                        X26
                                               X27
                                                       X28
                                                               X29
 X31
         X32
                 X33
                        X34
                                X35
                                        X36
                                               X37
                                                       X38
                                                               X39
 X41
         X42
                 X43
                        X44
                                X45
                                        X46
                                               X47
                                                       X48
                                                               X49
                        X54
                                X55
                                        X56
                                               X57
                                                       X58
                                                               X59
         X62
 X<sub>61</sub>
                 X63
                        X64
                                X<sub>65</sub>
                                        X66
                                               X67
                                                       X68
                                                               X69
X<sub>71</sub>
         X72
                 X73
                         X74
                                X75
                                        X76
                                                X77
                                                        X78
  X81
         X82
                 X83
                         X84
                                X85
                                        X86
                                                X87
                                                        X88
  X91
         X92
                 X93
                         X94
                                X95
                                        X96
                                                X97
                                                        X98
```

Processors = 0 1 2 3 4 5



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GBD: Example 2

# Understanding GBD: Non-Balanced GBD

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$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} & X_{15} & X_{16} & X_{17} & X_{18} & X_{19} \\ X_{21} & X_{22} & X_{23} & X_{24} & X_{25} & X_{26} & X_{27} & X_{28} & X_{29} \\ X_{31} & X_{32} & X_{33} & X_{34} & X_{35} & X_{36} & X_{37} & X_{38} & X_{39} \\ X_{41} & X_{42} & X_{43} & X_{44} & X_{45} & X_{46} & X_{47} & X_{48} & X_{49} \\ \hline X_{51} & X_{52} & X_{53} & X_{54} & X_{55} & X_{56} & X_{57} & X_{58} & X_{59} \\ X_{61} & X_{62} & X_{63} & X_{64} & X_{65} & X_{66} & X_{67} & X_{68} & X_{69} \\ \hline X_{71} & X_{72} & X_{73} & X_{74} & X_{75} & X_{76} & X_{77} & X_{78} & X_{79} \\ \hline X_{81} & X_{82} & X_{83} & X_{84} & X_{85} & X_{86} & X_{87} & X_{88} & X_{89} \\ X_{91} & X_{92} & X_{93} & X_{94} & X_{95} & X_{96} & X_{97} & X_{98} & X_{99} \end{bmatrix}$$

Processors = 0 1 2 3 4 5



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GBD: Example 2

```
Understanding GBD: Local View
                                                                                            \int_{0\times9}
                                                          X<sub>16</sub>
                                                                   X<sub>17</sub>
               X_{11}
                        X_{12}
                                X_{13}
                                         X_{14}
                                                 X_{15}
                                                                           X_{18}
                                                                                    X_{19}
               X21
                        X22
                                X23
                                         X24
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                                                          X26
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               X31
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                                                 X45
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               X<sub>41</sub>
                        X42
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                X51
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                                 X53
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                                                          X56
                                                                   X57
                                                                            X58
                                                                                    X59
                X<sub>61</sub>
                        X<sub>62</sub>
                                 X<sub>63</sub>
                                          X<sub>64</sub>
                                                  X<sub>65</sub>
                                                           X<sub>66</sub>
                                                                   X67
                                                                            X<sub>68</sub>
                                                                                    X69
                X71
                        X72
                                 X73
                                                                            X78
                                                                                     X79
                                          X74
                                                  X75
                                                           X76
                                                                   X77
                                                                                            ∫0×9
                X<sub>81</sub>
                        X82
                                 X83
                                                  X85
                                                           X86
                                                                   X87
                                                                            X88
                        X92
                X91
                                 X93
                                          X94
                                                  X95
                                                           X96
                                                                   X97
                                                                            X98
                                                                                     X99
                           Processors =
                                                   0
                                                                   3
```



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GBD: Example 2

## Quick Comment for GBD

Local pieces of GBD distributed objects will be given the suffix .gbd to visually help distinguish them from global objects. This suffix carries no semantic meaning.



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# **Brief Intermission**

## **Brief Intermission**

# Questions? Comments?

Don't forget to talk to us at our discussion group: http://group.r-pbd.org/

If you have an affiliation at a United States institution (university, research lab, etc.), consider getting an allocation with us: http://www.nics.tennessee.edu/getting-an-allocation

Come to the talk *Elevating R to Supercomputers*, Friday, July 12th at 10:00 at the High Performance Computing session



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  - pbdMPI Example: Sample Covariance
  - pbdMPI Example: Linear Regression



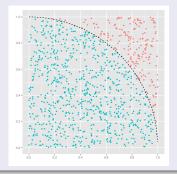
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pbdMPI Example: Monte Carlo Simulation

## Example 1: Monte Carlo Simulation

Sample *N* uniform observations  $(x_i, y_i)$  in the unit square  $[0, 1] \times [0, 1]$ . Then

$$\pi pprox 4\left(rac{\#\ \textit{Inside Circle}}{\#\ \textit{Total}}
ight) = 4\left(rac{\#\ \textit{Blue}}{\#\ \textit{Blue} + \#\ \textit{Red}}
ight)$$





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pbdMPI Example: Monte Carlo Simulation

# Example 1: Monte Carlo Simulation GBD Algorithm

- Let n be big-ish; we'll take n = 50,000.
- **2** Generate an  $n \times 2$  matrix x of standard uniform observations.
- **3** Count the number of rows satisfying  $x^2 + y^2 \le 1$
- Ask everyone else what their answer is; sum it all up.
- $\odot$  Take this new answer, multiply by 4 and divide by n
- o If my rank is 0, print the result.



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pbdMPI Example: Monte Carlo Simulation

## Example 1: Monte Carlo Simulation Code

#### Serial Code

```
1 N <- 50000
2 X <- matrix(runif(N * 2), ncol=2)
3 r <- sum(rowSums(X^2) <= 1)
4 PI <- 4*r/N
5 print(PI)</pre>
```

#### Parallel Code

```
library(pbdMPI, quiet = TRUE)
init()
comm.set.seed(diff=TRUE)

N.gbd <- 50000 / comm.size()
X.gbd <- matrix(runif(N.gbd * 2), ncol = 2)
r.gbd <- sum(rowSums(X.gbd^2) <= 1)
r <- allreduce(r.gbd)
PI <- 4*r/(N.gbd * comm.size())
comm.print(PI)
in print(PI)
in pri
```



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pbdMPI Example: Monte Carlo Simulation

## Note

For the remainder, we will exclude loading, init, and finalize calls.



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pbdMPI Example: Sample Covariance

## Example 2: Sample Covariance

$$cov(x_{n \times p}) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \mu_x) (x_i - \mu_x)^T$$



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pbdMPI Example: Sample Covariance

## Example 2: Sample Covariance GBD Algorithm

- $\bullet$  Determine the total number of rows N.
- 2 Compute the vector of column means of the full matrix.
- Subtract each column's mean from that column's entries in each local matrix.
- Ompute the crossproduct locally and reduce.
- **5** Divide by N-1.



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pbdMPI Example: Sample Covariance

# Example 2: Sample Covariance Code

## Serial Code

```
1  N <- nrow(X)
2  mu <- colSums(X) / N
3
4  X <- sweep(X, STATS=mu, MARGIN=2)
5  Cov.X <- crossprod(X) / (N-1)
6
7  print(Cov.X)</pre>
```

#### Parallel Code

```
1 N <- allreduce(nrow(X.gbd), op="sum")
2 mu <- allreduce(colSums(X.gbd) / N, op="sum")
3 
4 X.gbd <- sweep(X.gbd, STATS=mu, MARGIN=2)
5 Cov.X <- allreduce(crossprod(X.gbd), op="sum") / (N-1)
6 
7 comm.print(Cov.X)</pre>
```



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pbdMPI Example: Linear Regression

# Example 3: Linear Regression

Find  $\beta$  such that

$$\mathsf{y} = \mathsf{X} oldsymbol{eta} + \epsilon$$

When X is full rank,

$$\hat{oldsymbol{eta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$



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pbdMPI Example: Linear Regression

# Example 3: Linear Regression GBD Algorithm

- Locally, compute  $tx = x^T$
- 2 Locally, compute A = tx \* x. Query every other processor for this result and sum up all the results.
- **3** Locally, compute B = tx \* y. Query every other processor for this result and sum up all the results.
- **1** Locally, compute  $A^{-1} * B$



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pbdMPI Example: Linear Regression

# Example 3: Linear Regression Code

#### Serial Code

```
1 tX <- t(X)
2 A <- tX %*% X
3 B <- tX %*% y
4 ols <- solve(A) %*% B
```

#### Parallel Code



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Introduction to Distributed Matrices

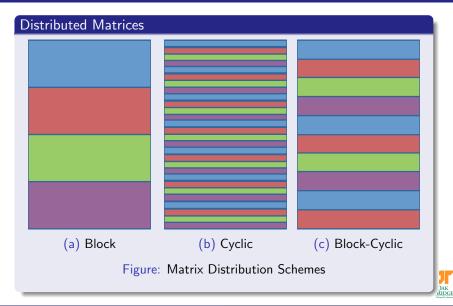
### Distributed Matrices

Most problems in data science are matrix algebra problems

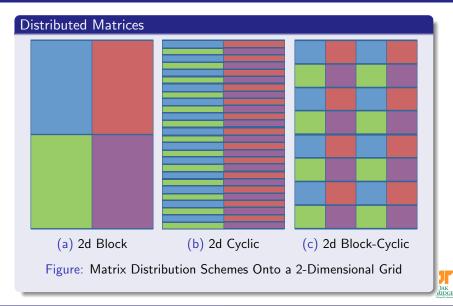
- Data structure: block-cyclic matrix distributed across a 2-dimensional grid of processors.
- No single processor should hold all of the data.
- Very robust, but very confusing data structure.



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# Processor Grid Shapes

$$\begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}^{T} \qquad \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 \\ 2 & 3 \\ 4 & 5 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 \\ 2 & 3 \\ 4 & 5 \end{bmatrix}$$
(a)  $1 \times 6$  (b)  $2 \times 3$  (c)  $3 \times 2$  (d)  $6 \times 1$ 

Table: Processor Grid Shapes with 6 Processors



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Introduction to Distributed Matrices

### Distributed Matrices

The data structure is a special R class (in the OOP sense) called ddmatrix. It is the "under the rug" storage for a block-cyclic matrix distributed onto a 2-dimensional processor grid.

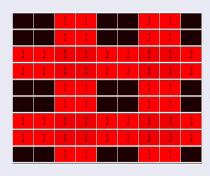
## with prototype

```
\label{eq:new("ddmatrix")} \text{new("ddmatrix")} = \begin{cases} \textbf{Data} &= \texttt{matrix}(0.0) \\ \textbf{dim} &= \texttt{c}(1,1) \\ \textbf{ldim} &= \texttt{c}(1,1) \\ \textbf{bldim} &= \texttt{c}(1,1) \\ \textbf{CTXT} &= 0.0 \end{cases}
```



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Example: an  $9 \times 9$  matrix is distributed with a "block-cycling" factor of  $2 \times 2$  on a  $2 \times 2$  processor grid:



$$= \begin{cases} \textbf{Data} &= \texttt{matrix}(...) \\ \textbf{dim} &= \texttt{c}(9, 9) \\ \textbf{Idim} &= \texttt{c}(...) \\ \textbf{bIdim} &= \texttt{c}(2, 2) \\ \textbf{CTXT} &= 0 \end{cases}$$

See http://acts.nersc.gov/scalapack/hands-on/datadist.html



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Introduction to Distributed Matrices

# Understanding Dmat: Global Matrix

$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} & X_{15} & X_{16} & X_{17} & X_{18} & X_{19} \\ X_{21} & X_{22} & X_{23} & X_{24} & X_{25} & X_{26} & X_{27} & X_{28} & X_{29} \\ X_{31} & X_{32} & X_{33} & X_{34} & X_{35} & X_{36} & X_{37} & X_{38} & X_{39} \\ X_{41} & X_{42} & X_{43} & X_{44} & X_{45} & X_{46} & X_{47} & X_{48} & X_{49} \\ X_{51} & X_{52} & X_{53} & X_{54} & X_{55} & X_{56} & X_{57} & X_{58} & X_{59} \\ X_{61} & X_{62} & X_{63} & X_{64} & X_{65} & X_{66} & X_{67} & X_{68} & X_{69} \\ X_{71} & X_{72} & X_{73} & X_{74} & X_{75} & X_{76} & X_{77} & X_{78} & X_{79} \\ X_{81} & X_{82} & X_{83} & X_{84} & X_{85} & X_{86} & X_{87} & X_{88} & X_{89} \\ X_{91} & X_{92} & X_{93} & X_{94} & X_{95} & X_{96} & X_{97} & X_{98} & X_{99} \end{bmatrix}$$



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## DMAT: 1-dimensional Row Block

$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} & X_{15} & X_{16} & X_{17} & X_{18} & X_{19} \\ X_{21} & X_{22} & X_{23} & X_{24} & X_{25} & X_{26} & X_{27} & X_{28} & X_{29} \\ X_{31} & X_{32} & X_{33} & X_{34} & X_{35} & X_{36} & X_{37} & X_{38} & X_{39} \\ \hline X_{41} & X_{42} & X_{43} & X_{44} & X_{45} & X_{46} & X_{47} & X_{48} & X_{49} \\ X_{51} & X_{52} & X_{53} & X_{54} & X_{55} & X_{56} & X_{57} & X_{58} & X_{59} \\ \hline X_{61} & X_{62} & X_{63} & X_{64} & X_{65} & X_{66} & X_{67} & X_{68} & X_{69} \\ \hline X_{71} & X_{72} & X_{73} & X_{74} & X_{75} & X_{76} & X_{77} & X_{78} & X_{79} \\ X_{81} & X_{82} & X_{83} & X_{84} & X_{85} & X_{86} & X_{87} & X_{88} & X_{89} \\ X_{91} & X_{92} & X_{93} & X_{94} & X_{95} & X_{96} & X_{97} & X_{98} & X_{99} \end{bmatrix}$$

Processor grid = 
$$\begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} (0,0) \\ (0,1) \\ (1,0) \\ (1,1) \end{bmatrix}$$



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## DMAT: 2-dimensional Row Block

$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} & X_{15} & X_{16} & X_{17} & X_{18} & X_{19} \\ X_{21} & X_{22} & X_{23} & X_{24} & X_{25} & X_{26} & X_{27} & X_{28} & X_{29} \\ X_{31} & X_{32} & X_{33} & X_{34} & X_{35} & X_{36} & X_{37} & X_{38} & X_{39} \\ X_{41} & X_{42} & X_{43} & X_{44} & X_{45} & X_{46} & X_{47} & X_{48} & X_{49} \\ X_{51} & X_{52} & X_{53} & X_{54} & X_{55} & X_{56} & X_{57} & X_{58} & X_{59} \\ \hline X_{61} & X_{62} & X_{63} & X_{64} & X_{65} & X_{66} & X_{67} & X_{68} & X_{69} \\ X_{71} & X_{72} & X_{73} & X_{74} & X_{75} & X_{76} & X_{77} & X_{78} & X_{79} \\ X_{81} & X_{82} & X_{83} & X_{84} & X_{85} & X_{86} & X_{87} & X_{88} & X_{89} \\ X_{91} & X_{92} & X_{93} & X_{94} & X_{95} & X_{96} & X_{97} & X_{98} & X_{99} \end{bmatrix}$$

Processor grid = 
$$\begin{vmatrix} 0 & 1 \\ 2 & 3 \end{vmatrix} = \begin{vmatrix} (0,0) & (0,1) \\ (1,0) & (1,1) \end{vmatrix}$$



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# DMAT: 1-dimensional Row Cyclic

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}$$

Processor grid = 
$$\begin{vmatrix} 0 \\ 1 \\ 2 \\ 3 \end{vmatrix} = \begin{vmatrix} (0,0) \\ (0,1) \\ (1,0) \\ (1.1) \end{vmatrix}$$



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Introduction to Distributed Matrices

# DMAT: 2-dimensional Row Cyclic

$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} & X_{15} & X_{16} & X_{17} & X_{18} & X_{19} \\ \hline X_{21} & X_{22} & X_{23} & X_{24} & X_{25} & X_{26} & X_{27} & X_{28} & X_{29} \\ \hline X_{31} & X_{32} & X_{33} & X_{34} & X_{35} & X_{36} & X_{37} & X_{38} & X_{39} \\ \hline X_{41} & X_{42} & X_{43} & X_{44} & X_{45} & X_{46} & X_{47} & X_{48} & X_{49} \\ \hline X_{51} & X_{52} & X_{53} & X_{54} & X_{55} & X_{56} & X_{57} & X_{58} & X_{59} \\ \hline X_{61} & X_{62} & X_{63} & X_{64} & X_{65} & X_{66} & X_{67} & X_{68} & X_{69} \\ \hline X_{71} & X_{72} & X_{73} & X_{74} & X_{75} & X_{76} & X_{77} & X_{78} & X_{79} \\ \hline X_{81} & X_{82} & X_{83} & X_{84} & X_{85} & X_{86} & X_{87} & X_{88} & X_{89} \\ \hline X_{91} & X_{92} & X_{93} & X_{94} & X_{95} & X_{96} & X_{97} & X_{98} & X_{99} \end{bmatrix}$$

Processor grid = 
$$\begin{vmatrix} 0 & 1 \\ 2 & 3 \end{vmatrix} = \begin{vmatrix} (0,0) & (0,1) \\ (1,0) & (1,1) \end{vmatrix}$$



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Introduction to Distributed Matrices

# DMAT: 2-dimensional Block-Cyclic

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}$$

Processor grid = 
$$\begin{vmatrix} 0 & 1 \\ 2 & 3 \end{vmatrix} = \begin{vmatrix} (0,0) & (0,1) \\ (1,0) & (1,1) \end{vmatrix}$$



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pbdDMAT

#### The DMAT Data Structure

The more complicated the processor grid, the more complicated the distribution.



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pbdDMAT

# DMAT: 2-dimensional Block-Cyclic with 6 Processors

$$X = \begin{bmatrix} X_{11} & X_{12} & X_{13} & X_{14} & X_{15} & X_{16} & X_{17} & X_{18} & X_{19} \\ X_{21} & X_{22} & X_{23} & X_{24} & X_{25} & X_{26} & X_{27} & X_{28} & X_{29} \\ X_{31} & X_{32} & X_{33} & X_{34} & X_{35} & X_{36} & X_{37} & X_{38} & X_{39} \\ X_{41} & X_{42} & X_{43} & X_{44} & X_{45} & X_{46} & X_{47} & X_{48} & X_{49} \\ X_{51} & X_{52} & X_{53} & X_{54} & X_{55} & X_{56} & X_{57} & X_{58} & X_{59} \\ X_{61} & X_{62} & X_{63} & X_{64} & X_{65} & X_{66} & X_{67} & X_{68} & X_{69} \\ X_{71} & X_{72} & X_{73} & X_{74} & X_{75} & X_{76} & X_{77} & X_{78} & X_{79} \\ X_{81} & X_{82} & X_{83} & X_{84} & X_{85} & X_{86} & X_{87} & X_{88} & X_{89} \\ X_{91} & X_{92} & X_{93} & X_{94} & X_{95} & X_{96} & X_{97} & X_{98} & X_{99} \end{bmatrix}$$

Processor grid = 
$$\begin{vmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{vmatrix} = \begin{vmatrix} (0,0) & (0,1) & (0,2) \\ (1,0) & (1,1) & (1,2) \end{vmatrix}$$



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pbdDMAT

# Understanding DMAT: Local View

X31

$$\begin{bmatrix} \frac{\mathsf{X}65}{\mathsf{X}95} & \frac{\mathsf{X}66}{\mathsf{X}96} \end{bmatrix}_{5\times 1}$$

$$\begin{bmatrix} x_{85} & x_{86} \end{bmatrix}_{4\times2}$$

Processor grid = 
$$\begin{vmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{vmatrix} = \begin{vmatrix} (0,0) & (0,1) & (0,2) \\ (1,0) & (1,1) & (1,2) \end{vmatrix}$$



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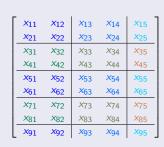
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pbdDMAT

#### The DMAT Data Structure

- DMAT is distributed. No one processor owns all of the matrix.
- ② DMAT is non-overlapping. Any piece owned by one processor is owned by no other processors.
- ① DMAT can be row-contiguous or not, depending on the processor grid and blocking factor used.
- OMAT is locally column-major and globally, it depends...
- GBD is a generalization of the one-dimensional block DMAT distribution. Otherwise there is no relation.
- O DMAT is confusing, but very robust.



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## Pros and Cons of This Data Structure

#### Pros

pbdDMAT

 Fast for distributed matrix computations

## Cons

Literally everything else

This is why we hide most of the distributed details.

The details are there if you want them (you don't want them).



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pbdDMAT

## Distributed Matrix Methods

**pbdDMAT** has over 100 methods with *identical* syntax to R:

- `[`, rbind(), cbind(), ...
- lm.fit(), prcomp(), cov(), ...
- `%\*%`, solve(), svd(), norm(), ...
- median(), mean(), rowSums(), ...

Serial Code

1 cov(x)

Parallel Code

1 cov(x)



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## Comparing pbdMPI and pbdDMAT

pbdDMAT

- **pbdMPI** is MPI + some sugar.
- The GBD data structure is not the only thing pbdMPI can handle (just a useful convention).
- **pbdDMAT** is more of a software package.
- The block-cyclic DMAT structure *must* be used for **pbdDMAT**.



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## Quick Comments for Using pbdDMAT

Start by loading the package:

```
library(pbdDMAT, quiet = TRUE)
```

② Always initialize before starting and finalize when finished:

```
init.grid()
3
  finalize()
```

Oistributed DMAT objects will be given the suffix .dmat to visually help distinguish them from global objects. This suffix carries no semantic meaning.



Statistics Examples with pbdDMAT

```
Sample Covariance

Serial Code

Cov.X <- cov(X)
print(Cov.X)

Parallel Code

Cov.X <- cov(X)
print(Cov.X)
```



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Statistics Examples with pbdDMAT

# Linear Regression

#### Serial Code

#### Parallel Code

```
1 tX <- t(X)
2 A <- tX %*% X
3 B <- tX %*% y
4
5 ols <- solve(A) %*% B
6
7 # or
8 ols <- lm.fit(X, y)</pre>
```



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#### Statistics Examples with pbdDMAT

#### Quick Example 3

#### PCA: pca.r

```
library(pbdDMAT, quiet=T)
    init.grid()
2
3
4
5
6
7
   n <- 1e4
   p <- 250
   comm. set . seed ( diff=T)
8
   x.dmat <- ddmatrix("rnorm", nrow=n, ncol=p, mean=100, sd=25)
10
    pca <- prcomp(x=x.dmat. retx=TRUE, scale=TRUE)</pre>
11
    prop_var <- cumsum(pca$sdev)/sum(pca$sdev)</pre>
12
    i \leftarrow max(min(which(prop_var > 0.9)) - 1, 1)
13
14
   y.dmat \leftarrow pcax[, 1:i]
15
   comm.cat("\nCols: ", i, "\n", quiet=T)
16
   comm. cat("\%Cols:", i/dim(x.dmat)[2], "\n\n", quiet=T)
17
18
19
    finalize()
```

#### Execute this script via:

Sample Output:

```
1 mpirun -np 2 Rscript pca.r 1 Cols: 221 %Cols: 0.884
```



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pbdDMAT Example: Generating Data

## Generating Random Data

Using randomly generated matrices is the best way to "get your feet wet" with the pbd tools. You can do this in 2 ways:

- Generate a global matrix and distribute it.
- 2 Generate locally only what is needed.



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pbdDMAT Example: Generating Data

# Example 1: Random Distributed Matrix Generation

## Generate a global matrix and distribute it

```
library(pbdDMAT, quiet=TRUE)
  init.grid()
3
  # Common global on all processors --> distributed
  comm.set.seed(diff=FALSE)
  x <- matrix(rnorm(100), nrow=10, ncol=10)
  x.dmat <- as.ddmatrix(x)
8
  # Global on processor 0 --> distributed
  if (comm.rank() == 0) {
10
    x <- matrix(rnorm(100), nrow=10, ncol=10)
11
12
  } else {
    x <- NULL
13
14
  x.dmat <- as.ddmatrix(x)
16
  finalize()
17
```



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pbdDMAT Example: Generating Data

# Example 2: Random Distributed Matrix Generation

Generate locally only what is needed

```
library(pbdDMAT, quiet=TRUE)
init.grid()

comm.set.seed(diff = TRUE) # good seeds via rlecuyer
x.dmat <- ddmatrix("rnorm", nrow=10, ncol=10)

finalize()</pre>
```



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pbdDMAT Example: Generating Data

# Example 3: Random Distributed Matrix Generation

Generate locally only what is needed

```
library(pbdDMAT, quiet=TRUE)
init.grid()

zero.dmat <- ddmatrix(0, nrow=100, ncol=100)
id.dmat <- diag(1, nrow=100, ncol=100)

finalize()</pre>
```



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# Example 4: Random Distributed Matrix Generation

#### Convert between GBD and DMAT

```
library(pbdDEMO, quiet=TRUE)
   init.grid()
3
   comm.set.seed(diff = TRUE)
5
   N.gbd \leftarrow 1 + comm.rank()
   X.gbd \leftarrow matrix(rnorm(N.gbd * 3), ncol = 3)
8
9
   # convert GBD to DMAT
   X.dmat <- gbd2dmat(X.gbd)</pre>
10
11
12
   # convert DMAT to GBD
13
   new.X.gbd <- dmat2gbd(X.dmat)</pre>
14
15
  # undistribute
  X <- as.matrix(X.dmat)</pre>
16
17
  finalize()
18
```



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0

pbdDMAT Example: Converting Between GBD and DMAT

#### Distributed Matrices

pbdDEMO contains many other examples of reading and managing GBD and DMAT data



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# Contents





### Where to Learn More

- Our website http://r-pbd.org/
- The pbdDEMO package
   http://cran.r-project.org/web/packages/pbdDEMO/
- The pbdDEMO Vignette: http://goo.gl/HZkRt
- Our Google Group: http://group.r-pbd.org



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# Thanks for coming!

Questions? Comments?

Don't forget to come to the talk:

Elevating R to Supercomputers
Friday, July 12th at 10:00
at the High Performance Computing session!



http://r-pbd.org pbdR Core Team Introduction to pbdR