pbdR: Programming with Big Data in R

pbdR Core Team

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The pbdR Core Team

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pbdR
Programming with Big Data in R

Support

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About This Presentation

Downloads

This presentation is available at:

https://github.com/wrathematics/pbd-tutorial/blob/master/pbdr/useR/pbdr.pdf?raw=true

Scripts for exercises are at:

https://github.com/wrathematics/pbd-tutorial/tree/master/pbdr/common/scripts

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*

http://goo.gl/HZkRt

It contains more examples, and sometimes added detail.

About This Presentation

Installation Instructions

Installation instructions for setting up a pbdR environment are available:

http://r-pbd.org/install.html

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

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Contents

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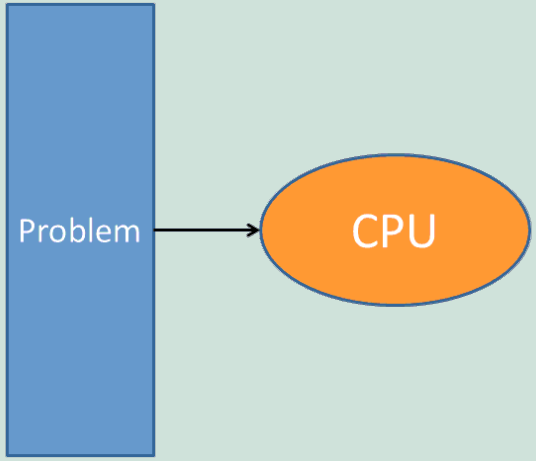
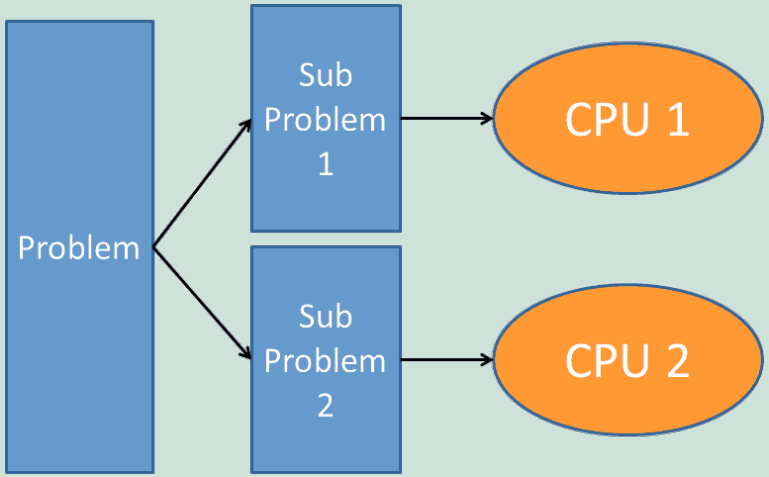
   - A Concise Introduction to Parallelism
   - Quick Overview of Parallel Hardware
   - A Quick Overview of Parallel Software
   - pbdR Connects R to HPC Libraries
   - Supercomputer and Parallel File System

Parallelism

Serial Programming

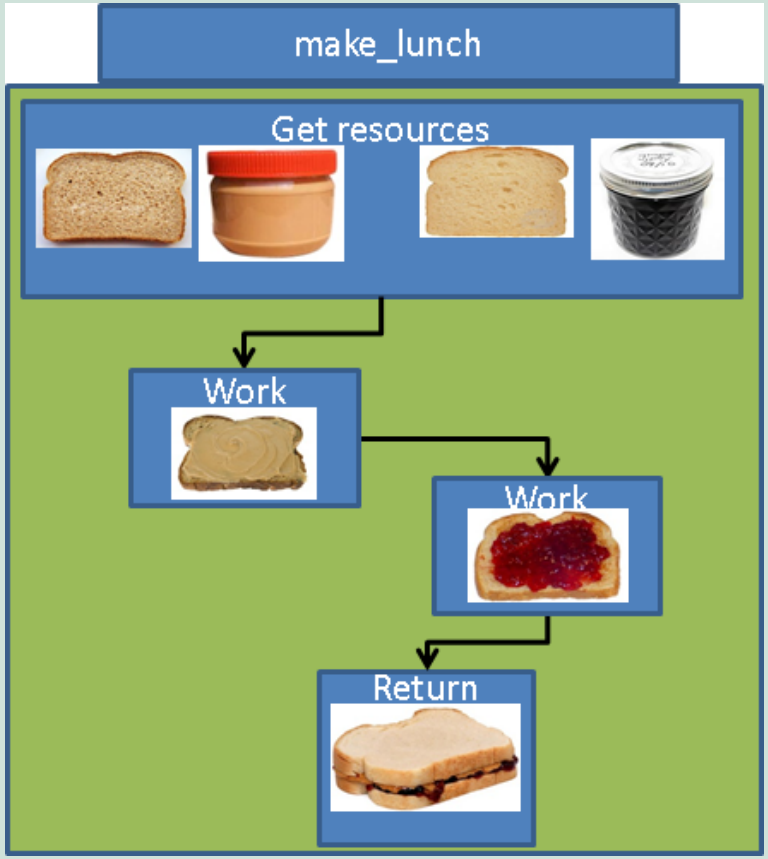


Parallel Programming

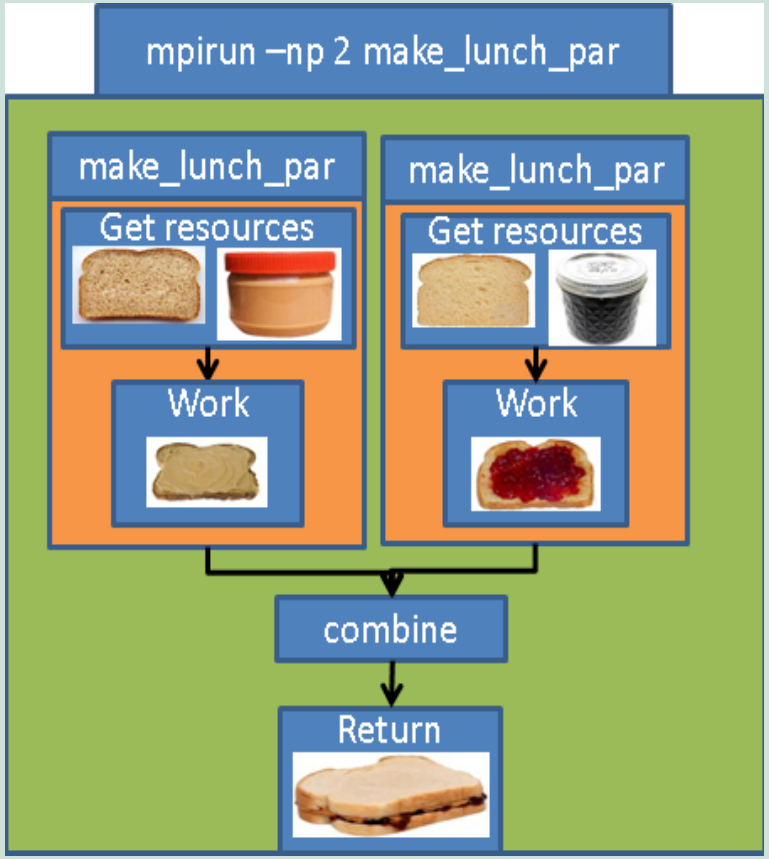


Parallelism

Serial Programming



Parallel Programming



Parallel Programming Vocabulary: Difficulty in Parallelism

1. *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.
4. *Tightly Coupled*: Opposite of embarrassingly parallel; lots of dependence in computations.

Speedup

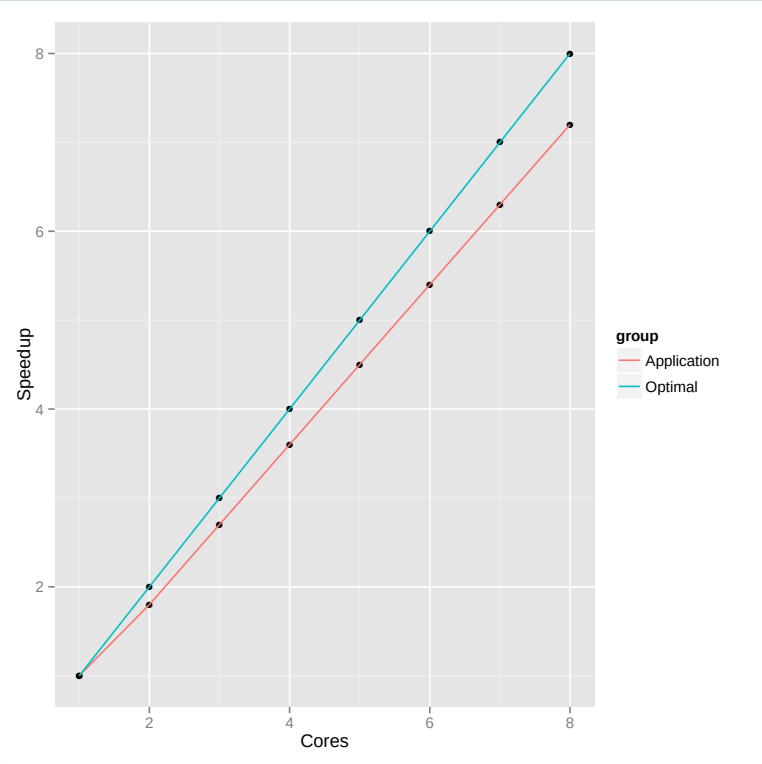
- *Wallclock Time*: Time of the clock on the wall from start to finish
- *Speedup*: unitless measure of improvement; more is better.

$$S_{n_1,n_2} = \frac{\text{Run time for } n_1 \text{ cores}}{\text{Run time for } n_2 \text{ cores}}$$

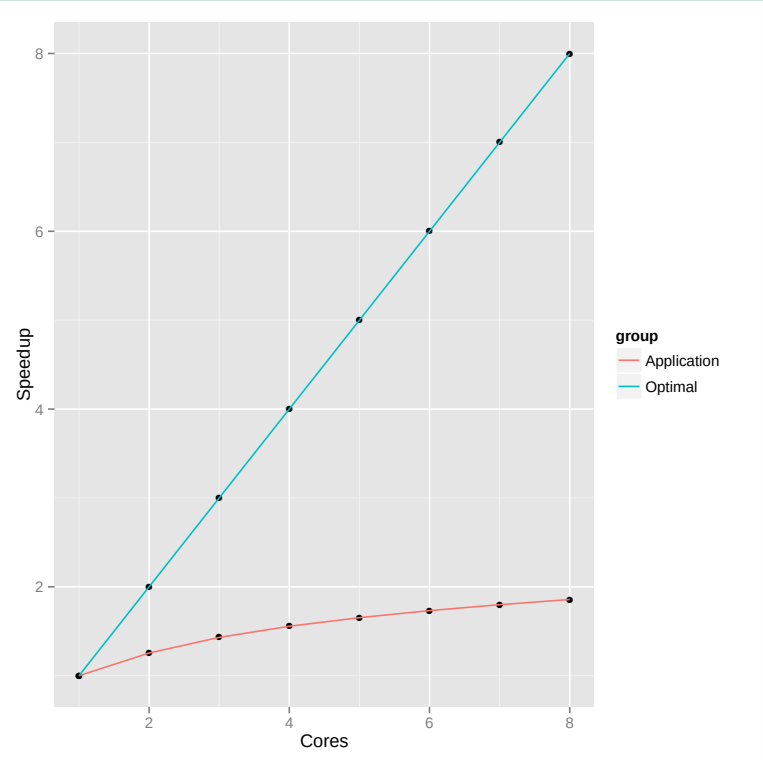
  - n_1 is often taken to be 1
  - In this case, comparing parallel algorithm to serial algorithm

Speedup

Good Speedup



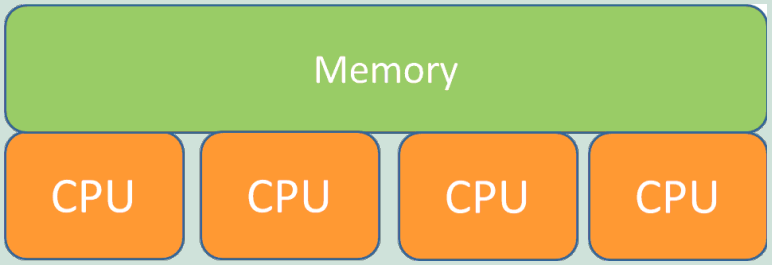
Bad Speedup



Shared and Distributed Memory Machines

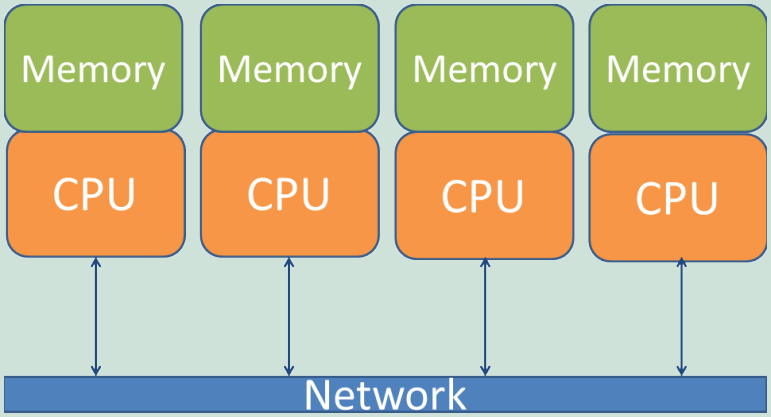
Shared Memory

Direct access to read/change memory (one node)



Distributed

No direct access to read/change memory (many nodes); requires communication



Shared and Distributed Memory Machines

Shared Memory Machines

Thousands of cores

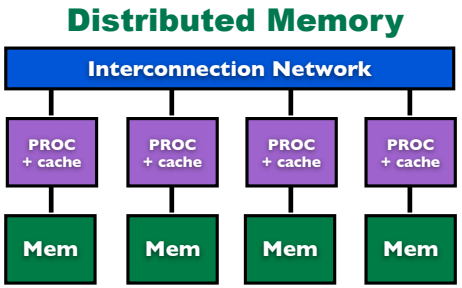
Nautilus, University of Tennessee
1024 cores
4 TB RAM

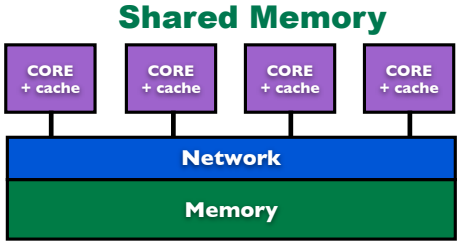
Distributed Memory Machines

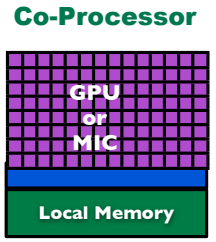
Hundreds of thousands of cores

Kraken, University of Tennessee
112,896 cores
147 TB RAM

Three Basic Flavors of Hardware



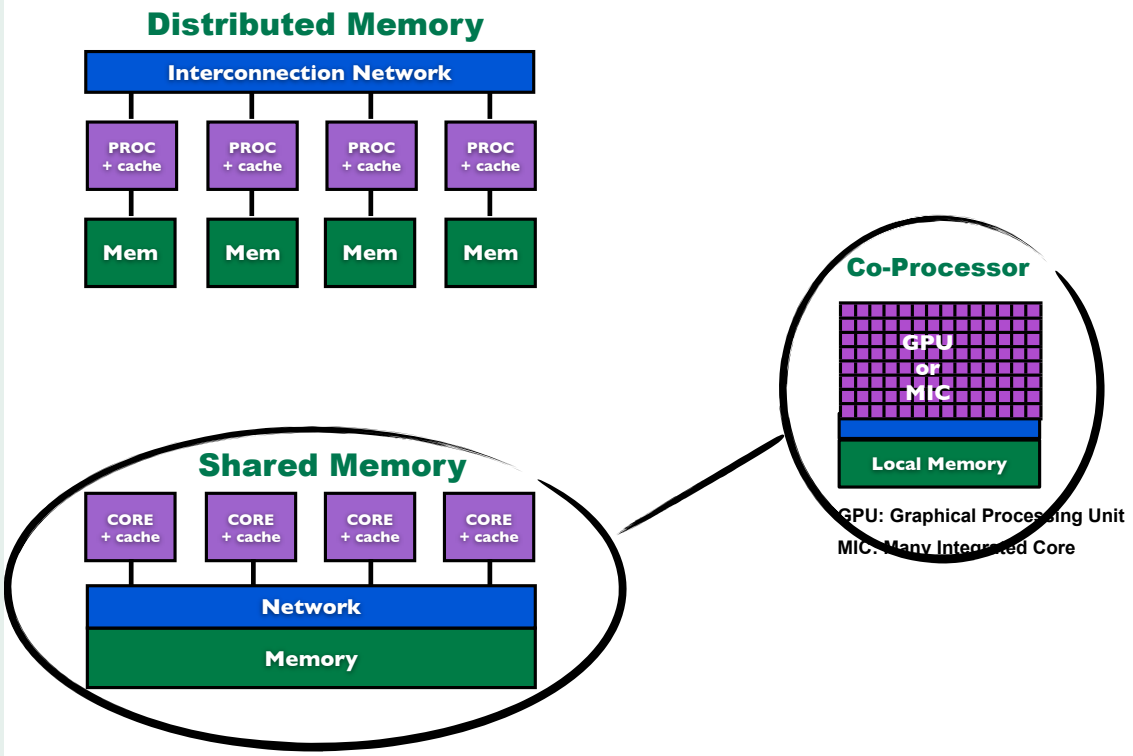




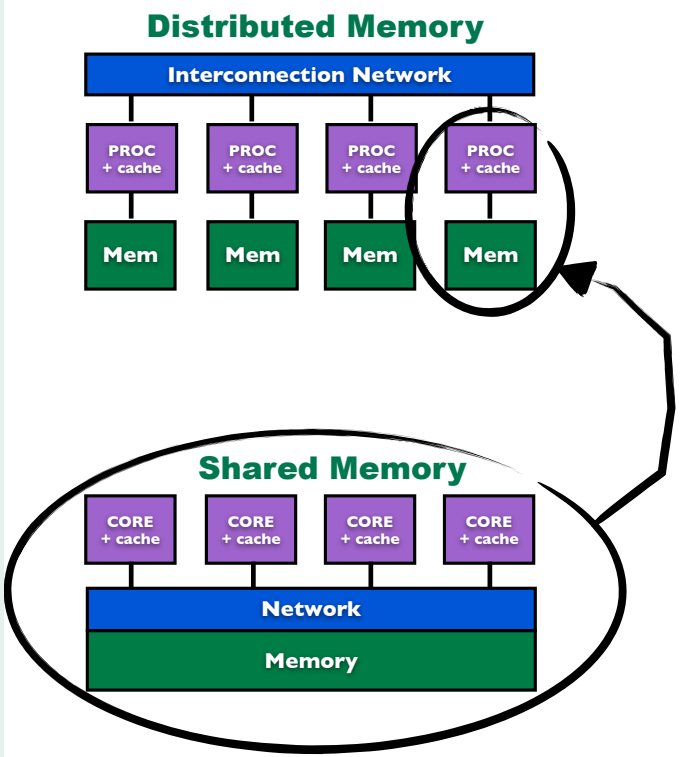
GPU: Graphical Processing Unit

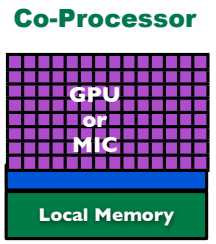
MIC: Many Integrated Core

Your Laptop or Desktop



A Server or Cluster

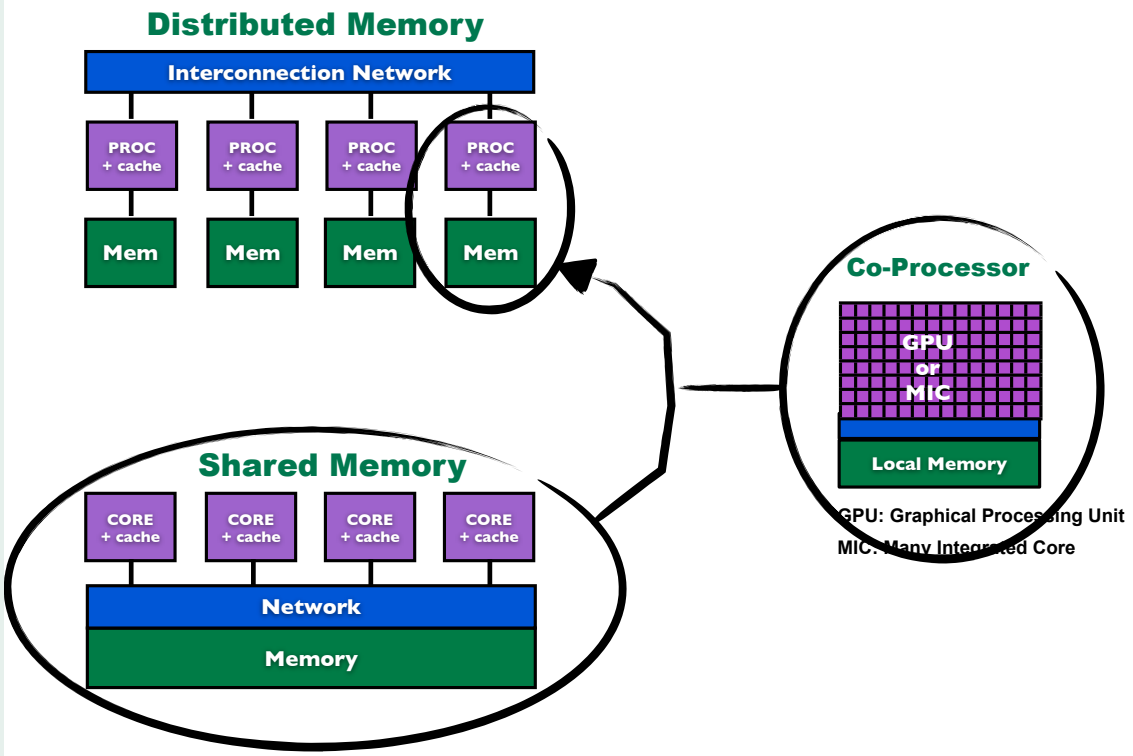




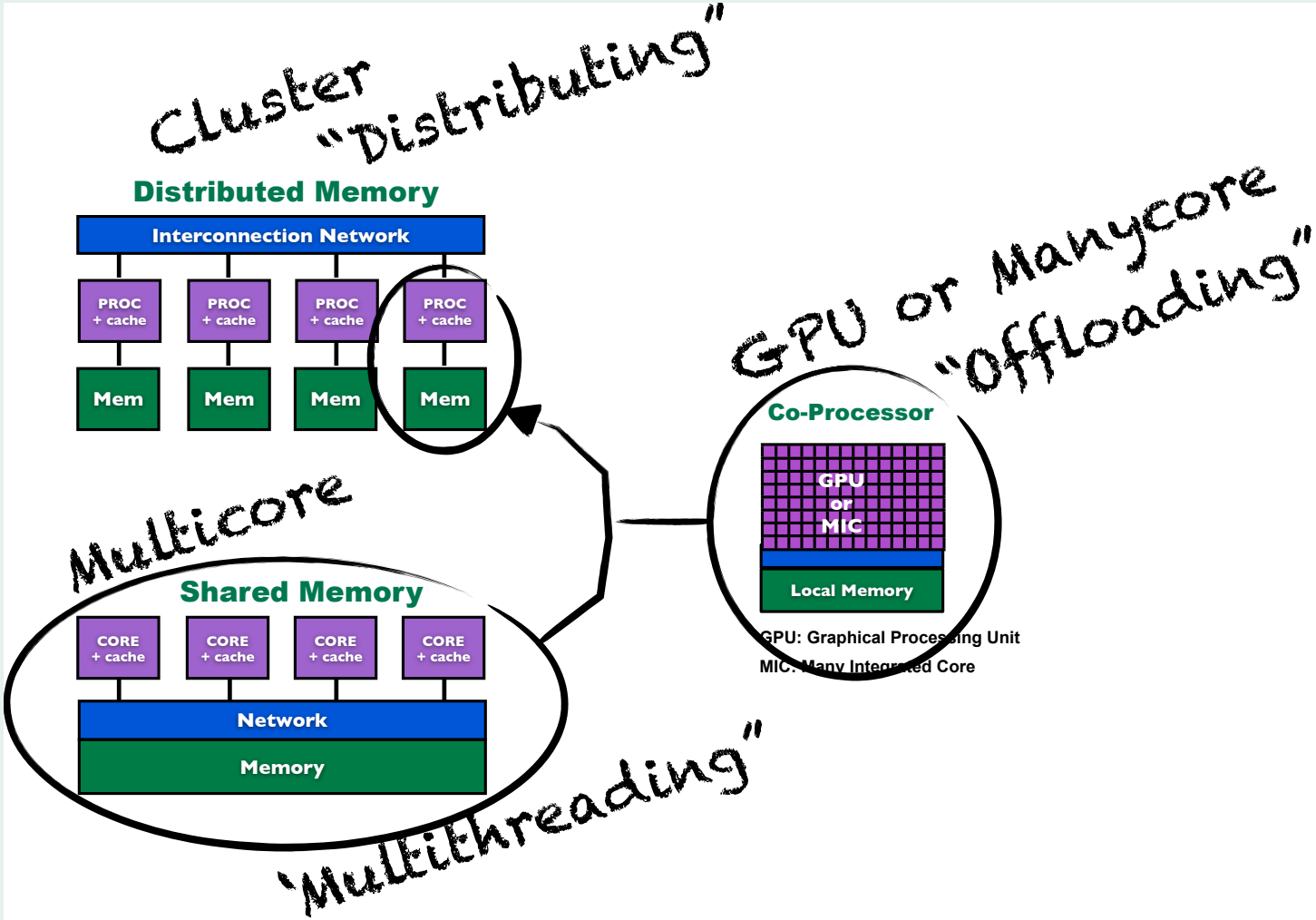
GPU: Graphical Processing Unit

MIC: Many Integrated Core

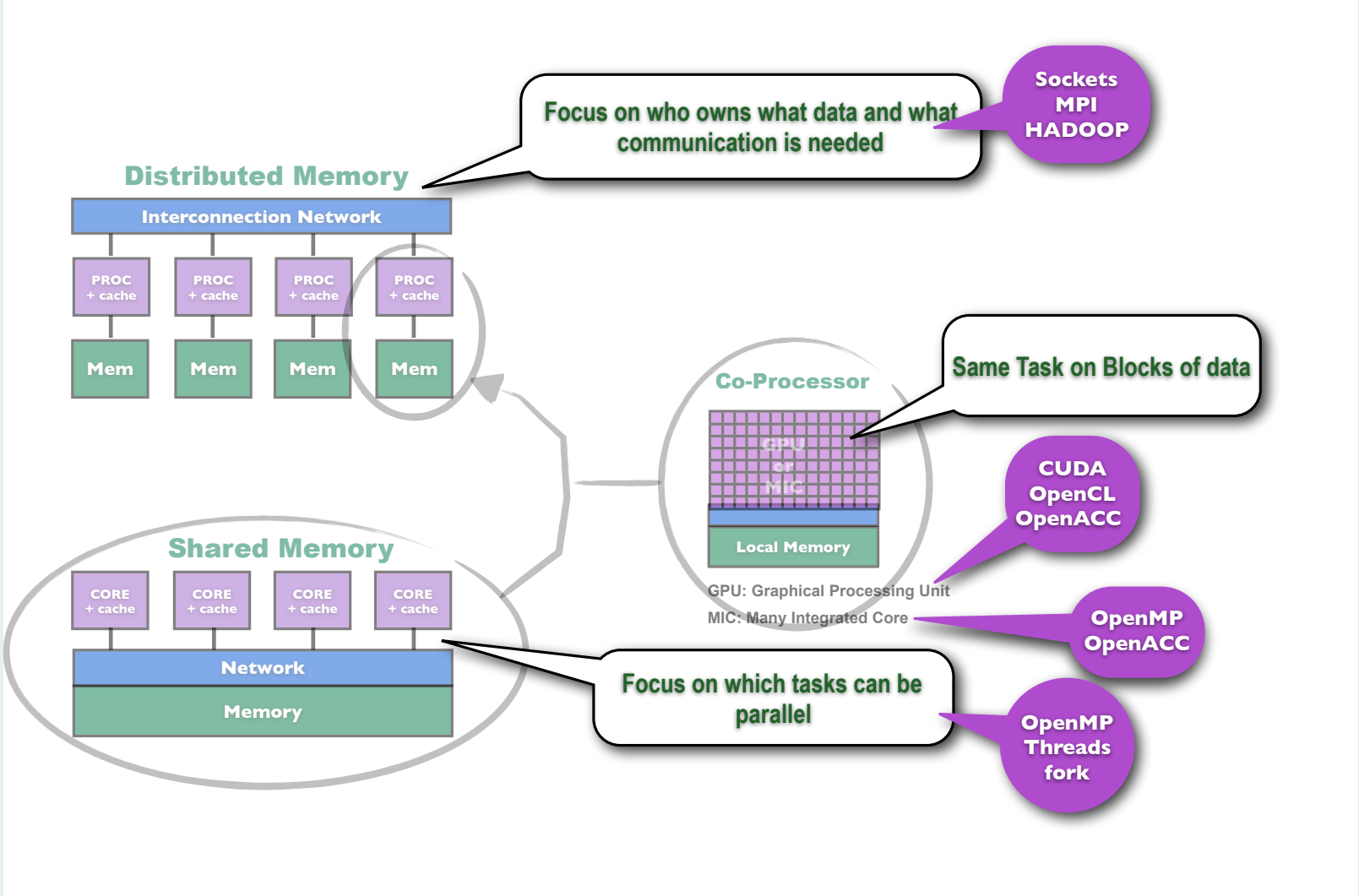
Server to Supercomputer



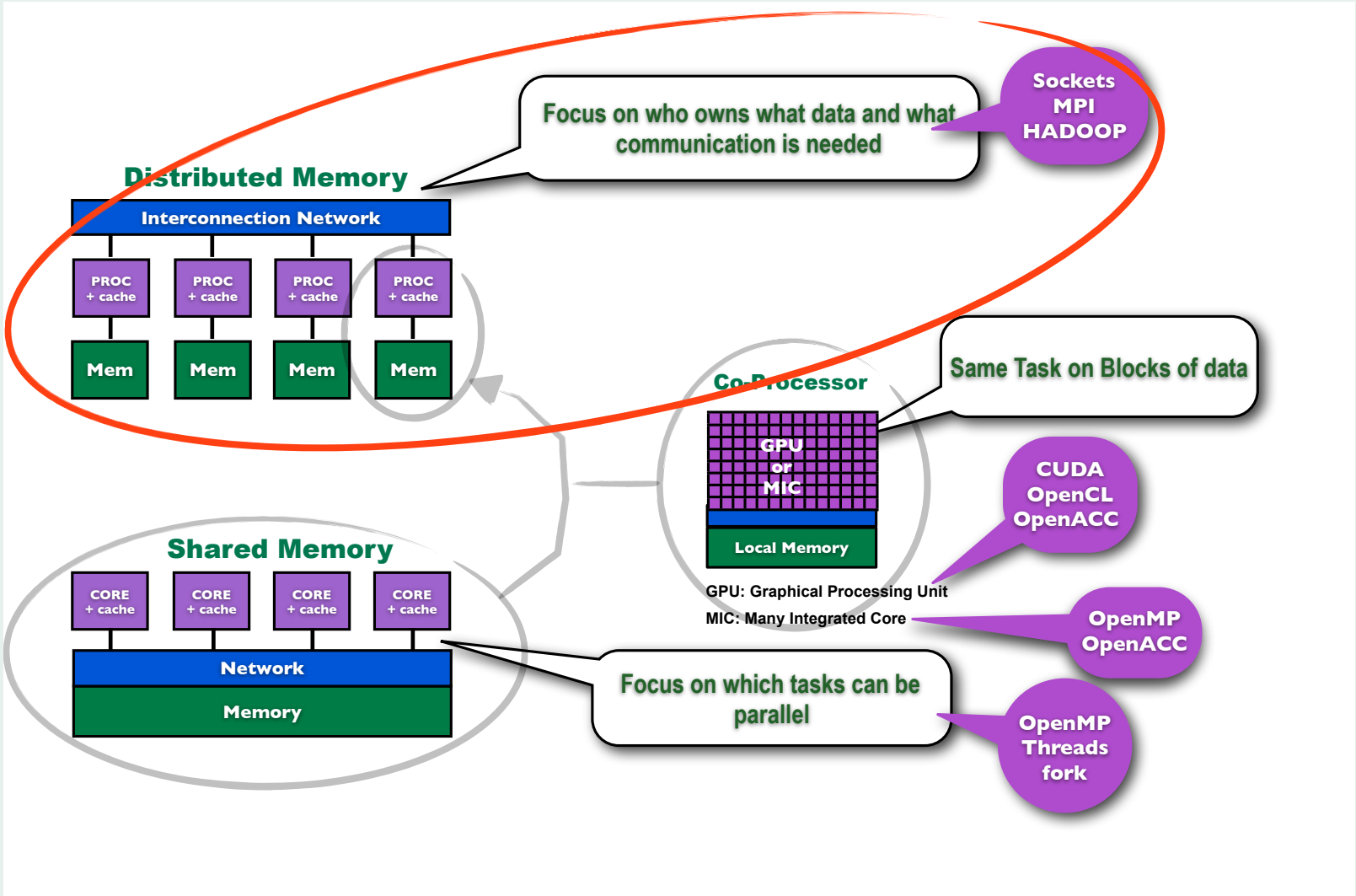
Knowing the Right Words



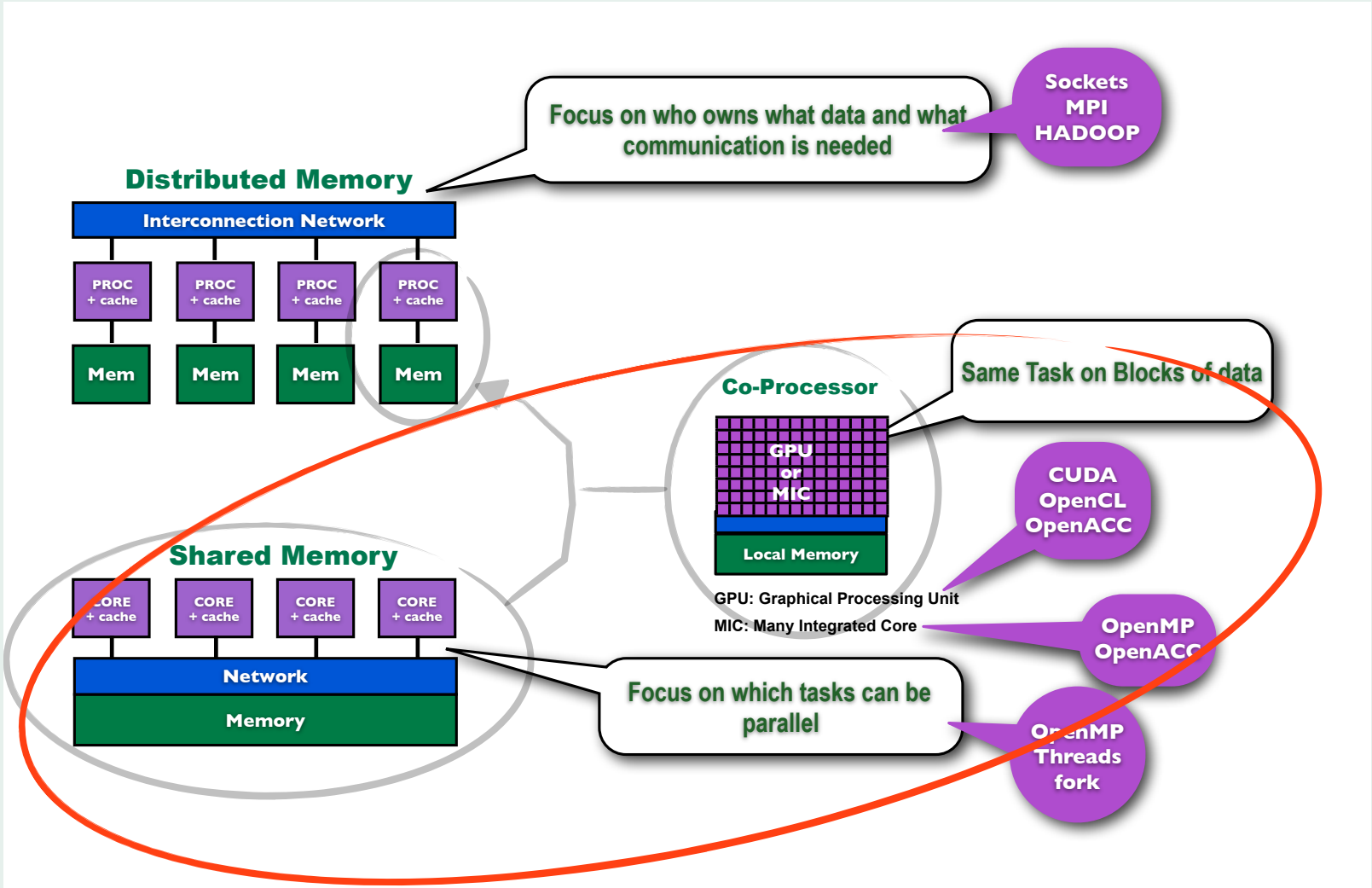
"Native" Programming Models and Tools



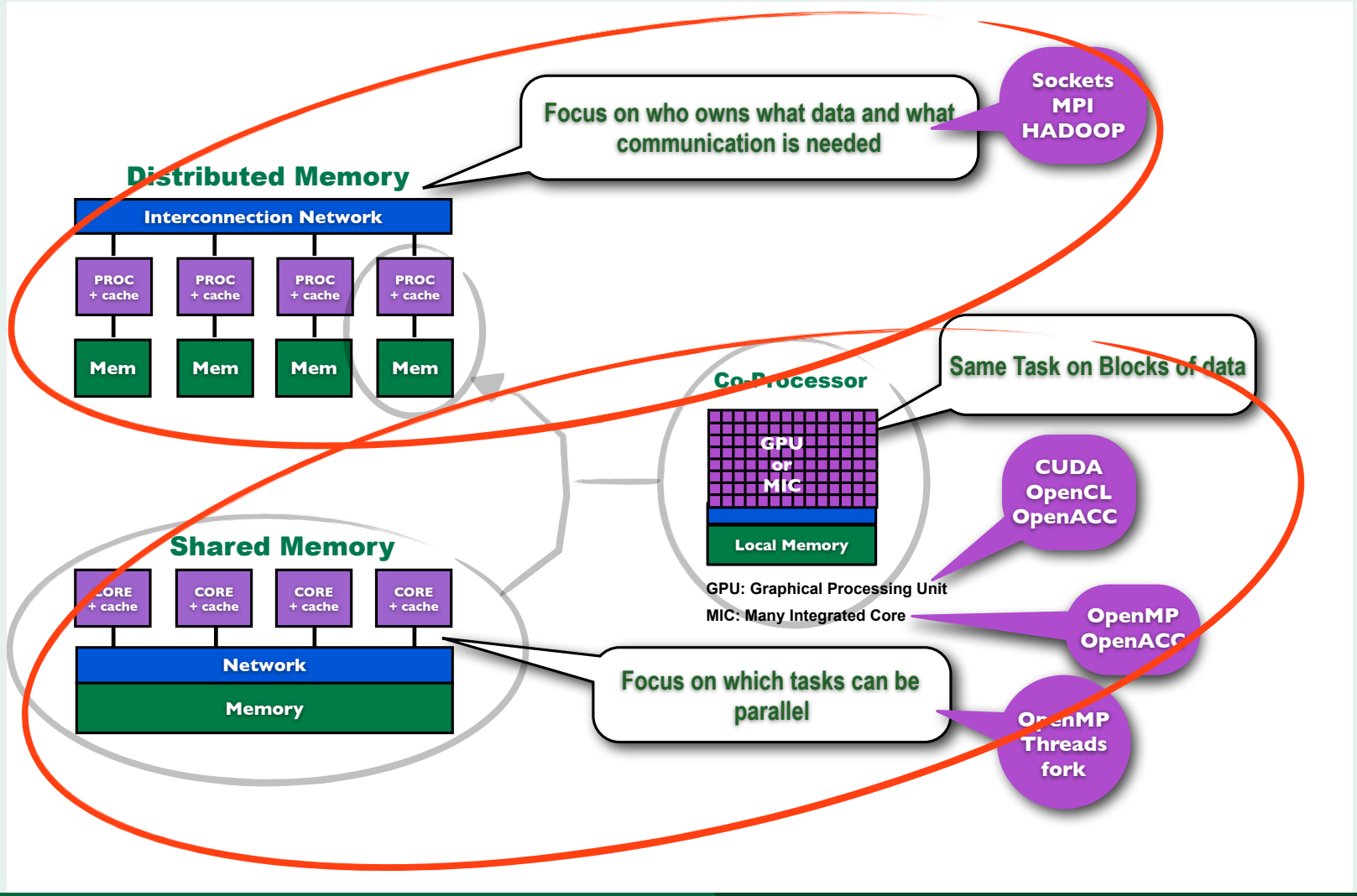
30+ Years of Parallel Computing Research



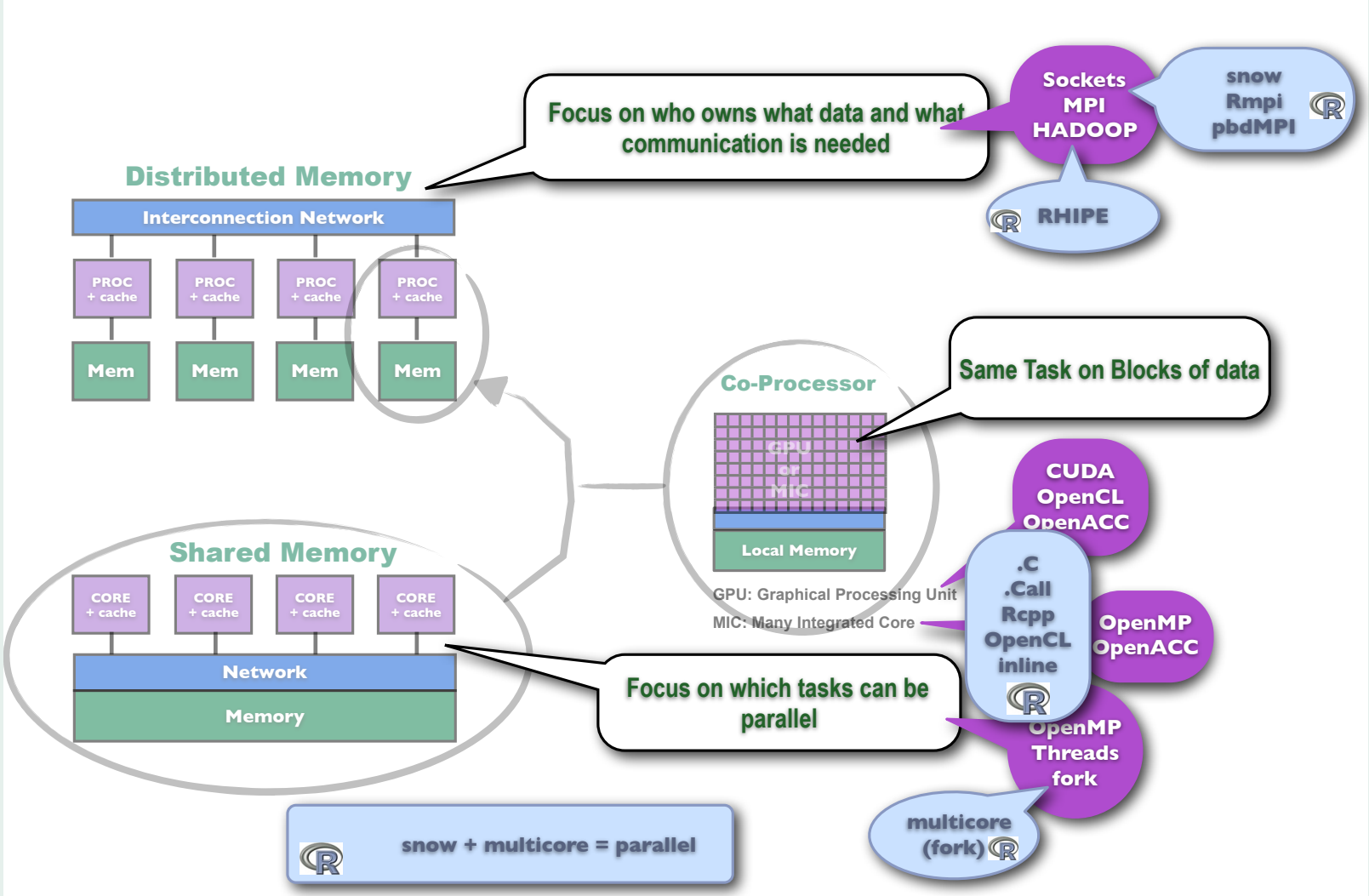
Last 10 years of Advances



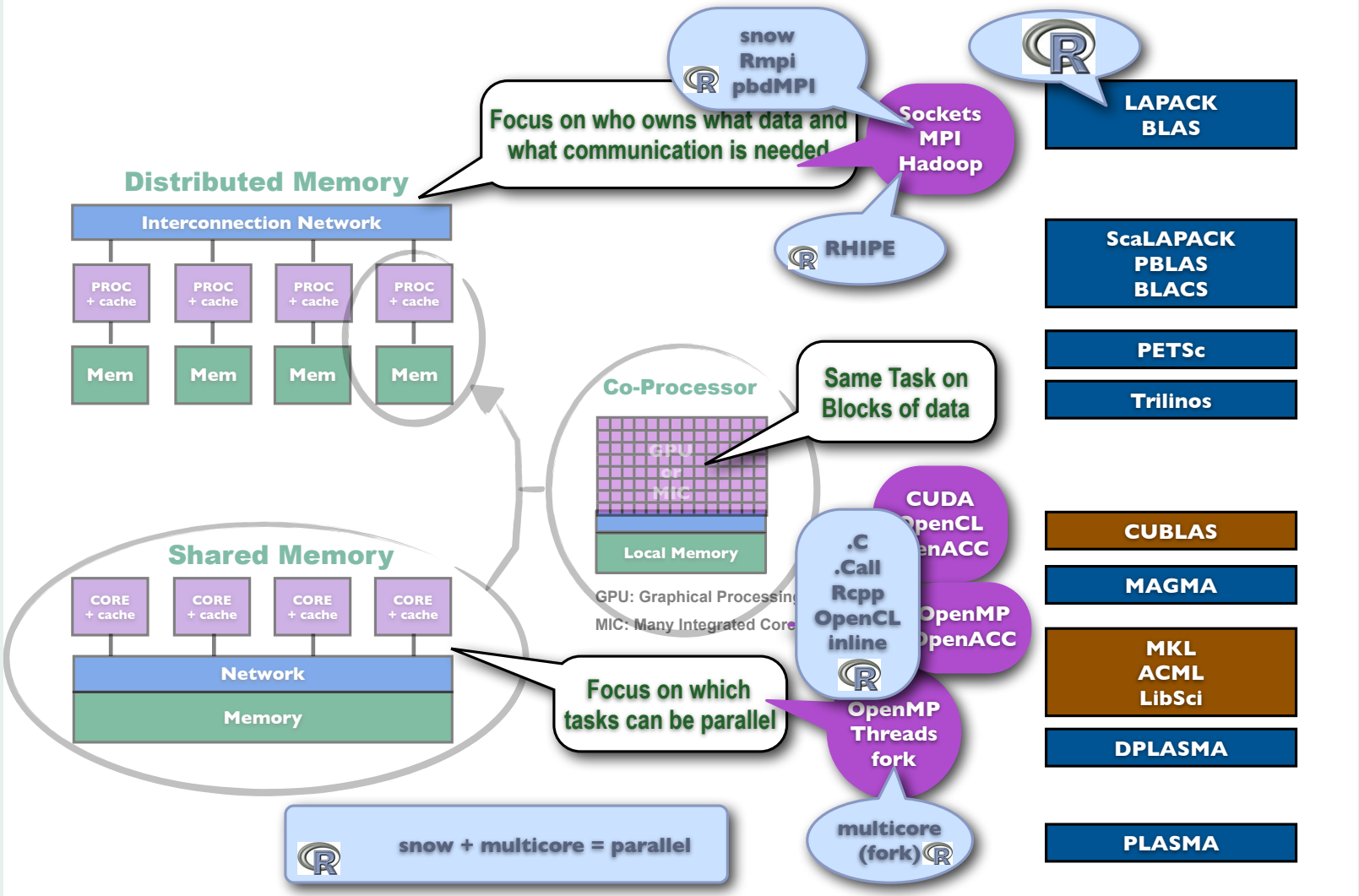
Putting It All Together Challenge



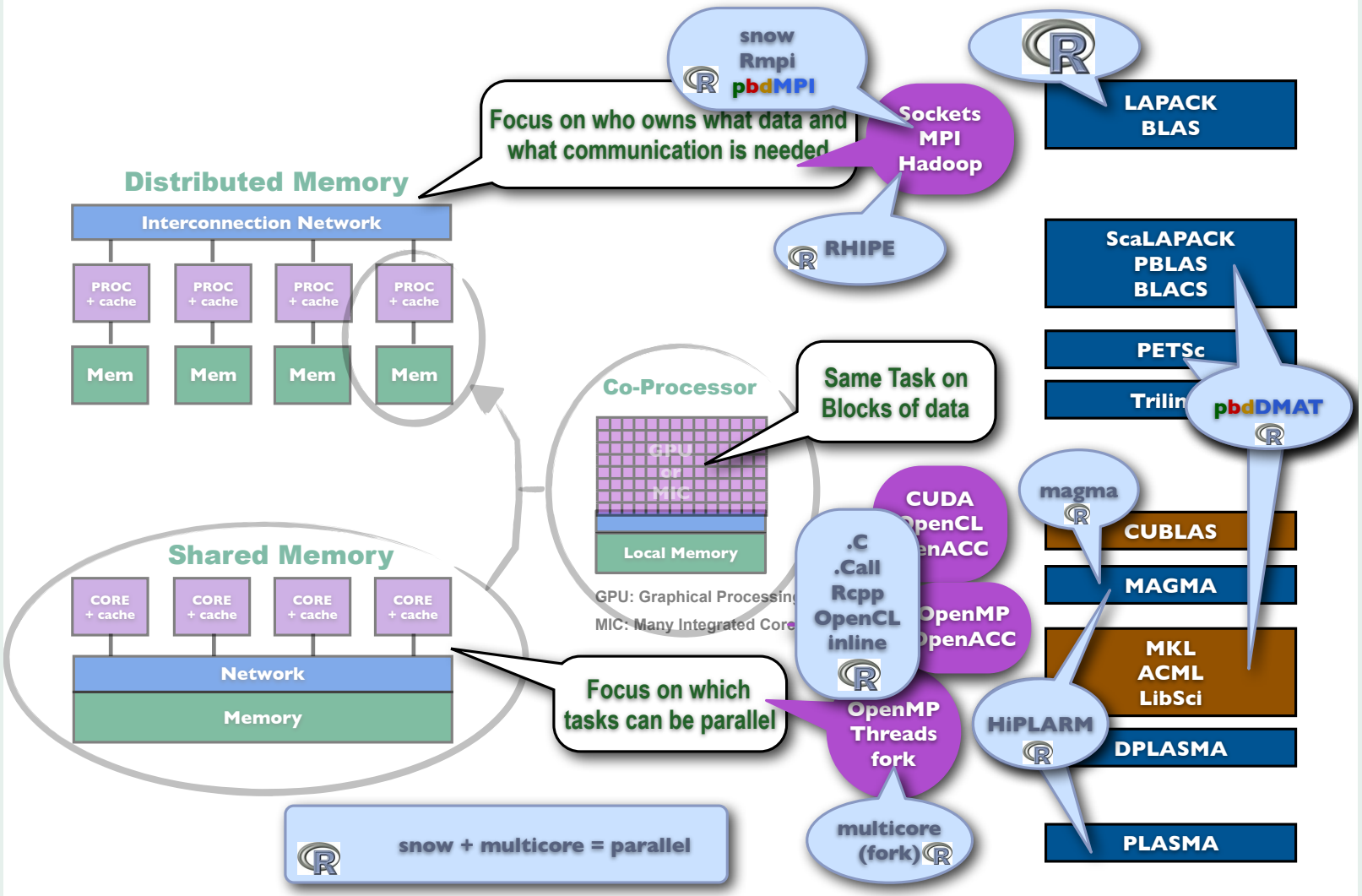
R Interfaces to Native Tools



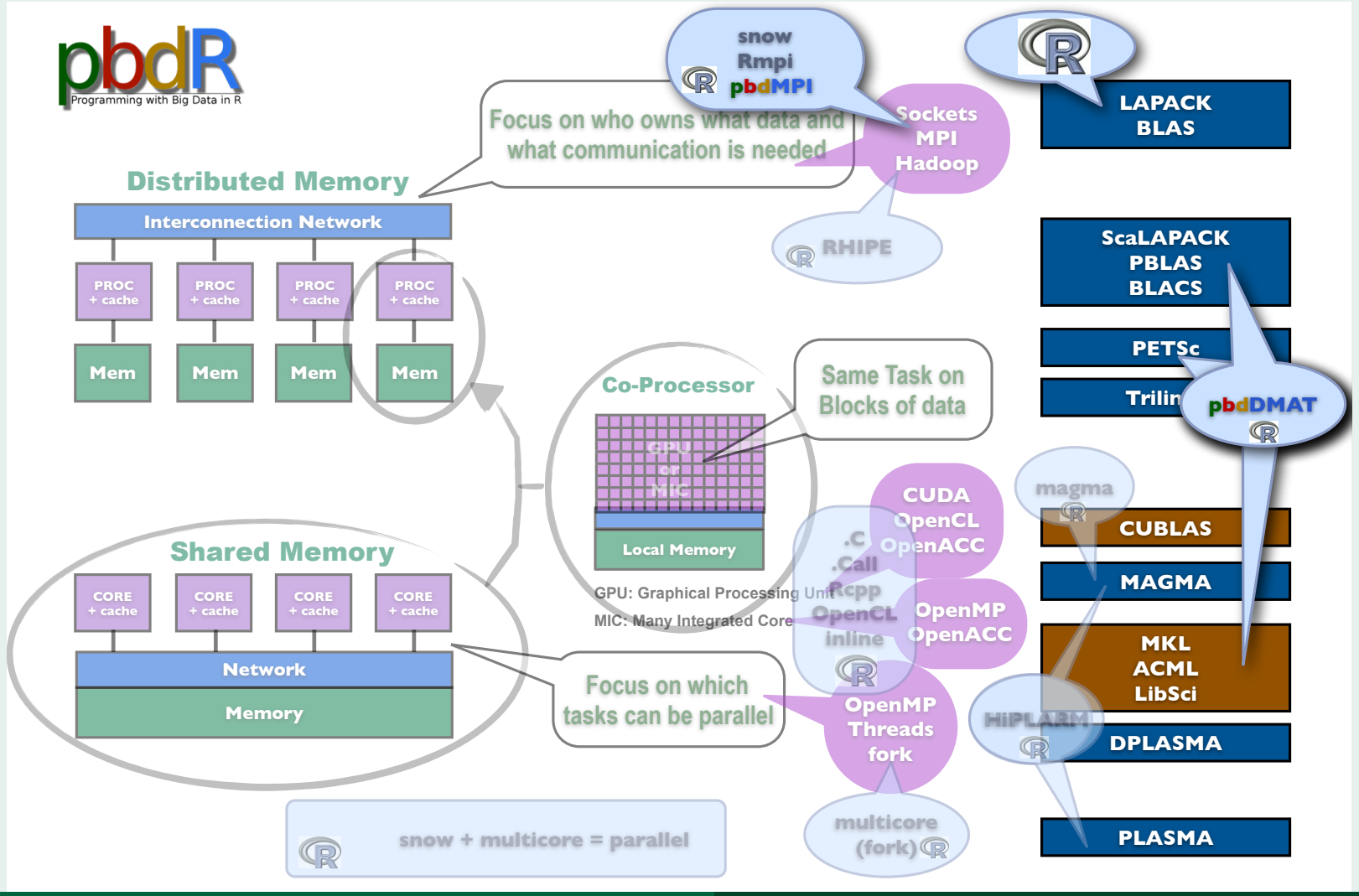
HPC Libraries



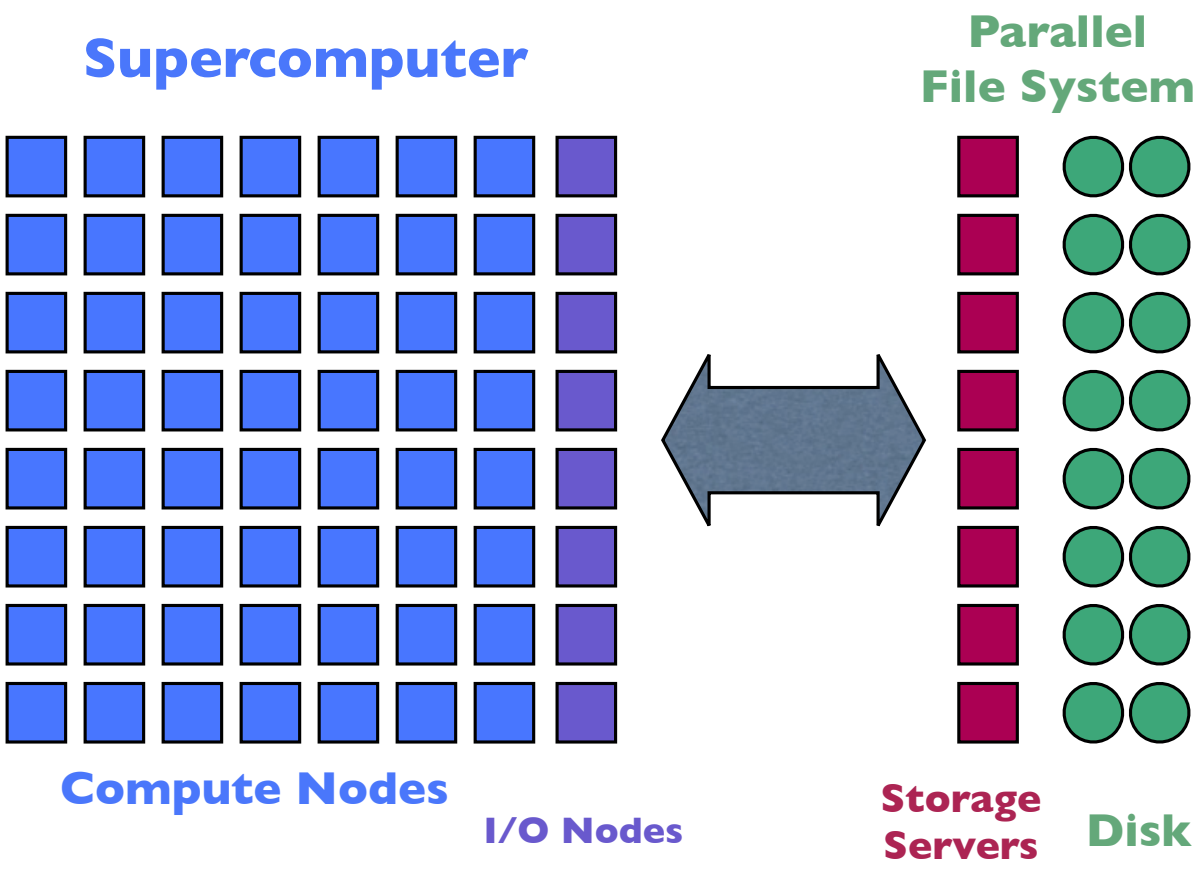
R Interfaces to Scalable HPC Libraries



pbdR Interfaces to Scalable HPC Libraries



Building R Infrastructure for Supercomputers



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- The pbdR Project
- Using pbdR

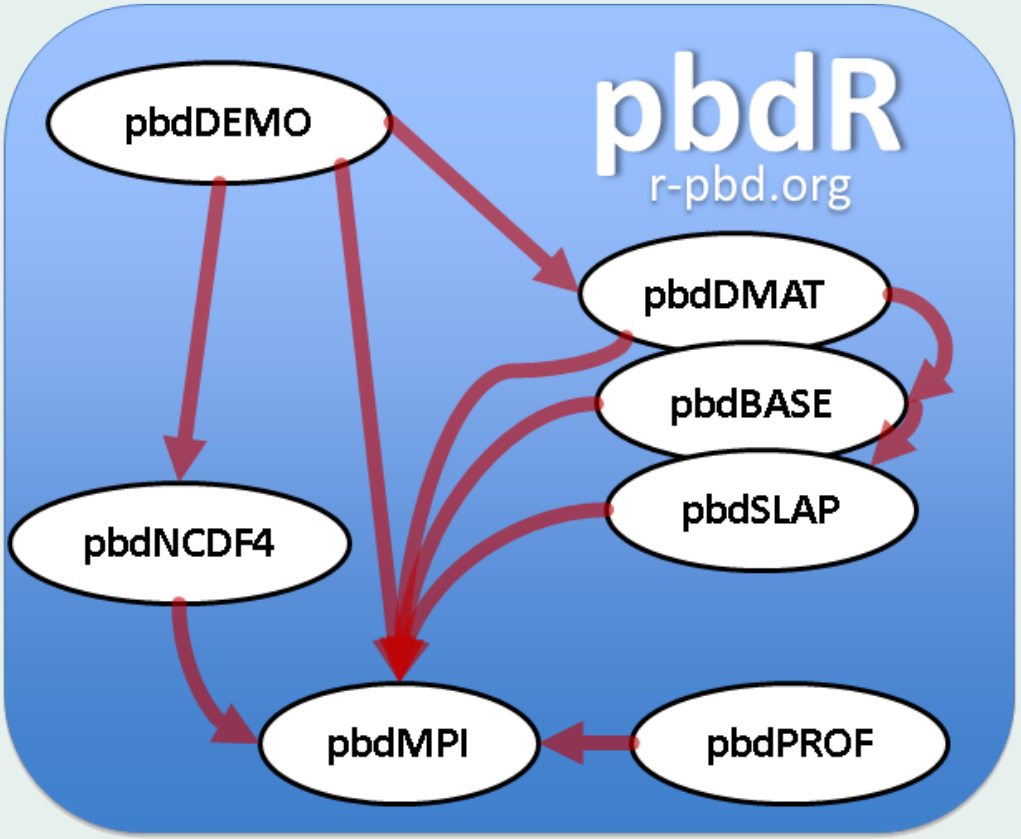
Programming with Big Data in R (pbdR)

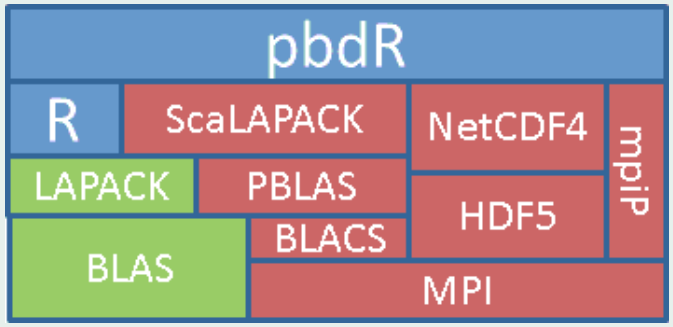
Striving for *Productivity, Portability, Performance*

- *Free*[a] R packages.
- Bridging high-performance compiled code with high-productivity of R
- Scalable, big data analytics.
- Offers implicit and explicit parallelism.
- Methods have syntax *identical* to R.

[a] MPL, BSD, and GPL licensed

pbdR Packages



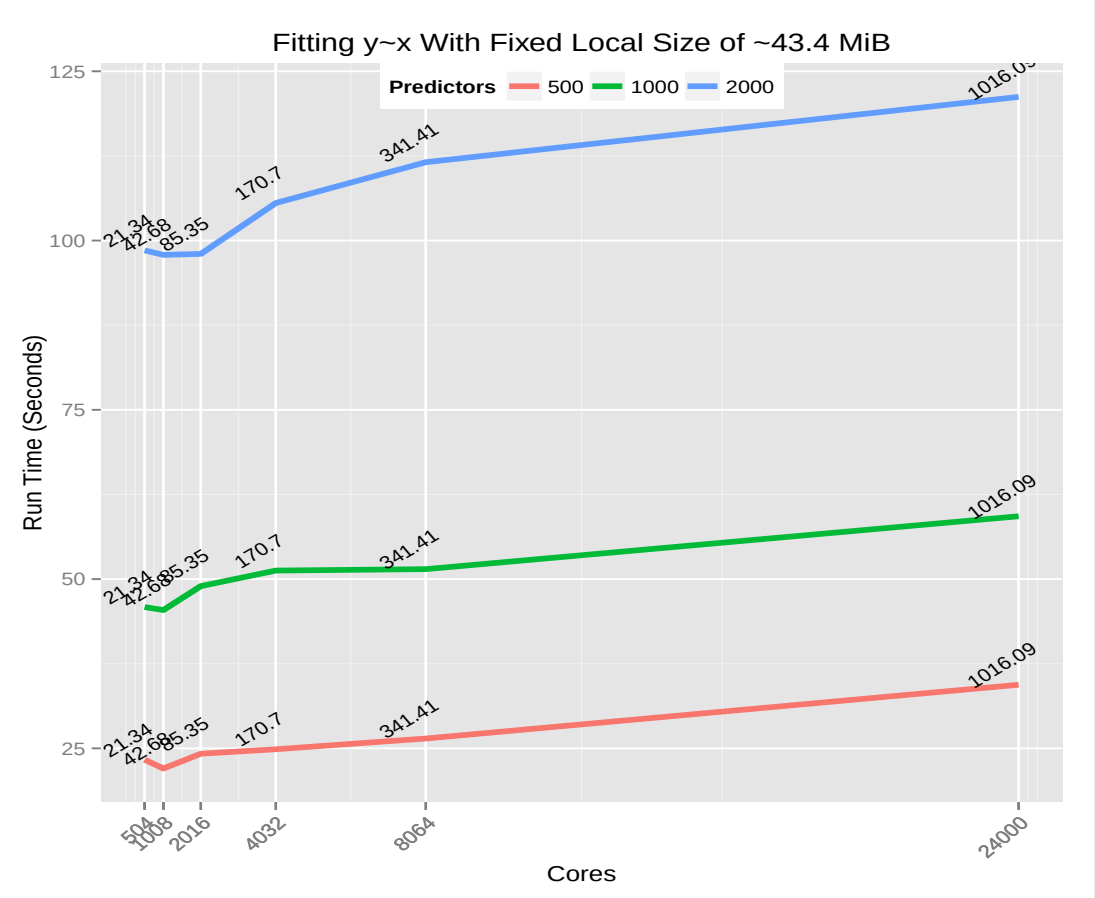


Simple, Intuitive MPI Operations with **pbdMPI**

Placeholder

Distributed Matrices and Statistics with **pbdDMAT**

Least Squares Benchmark




```
x <- ddmatrix("rnorm", nrow=m, ncol=n)
y <- ddmatrix( "rnorm", nrow=m, ncol=1)
```

Profiling with **pbdPROF**

1. Rebuild **pbdR** packages

```
R CMD INSTALL
    pbdMPI_0.2-1.tar.gz \
    --configure-args= \
    "--enable-pbdPROF"
```

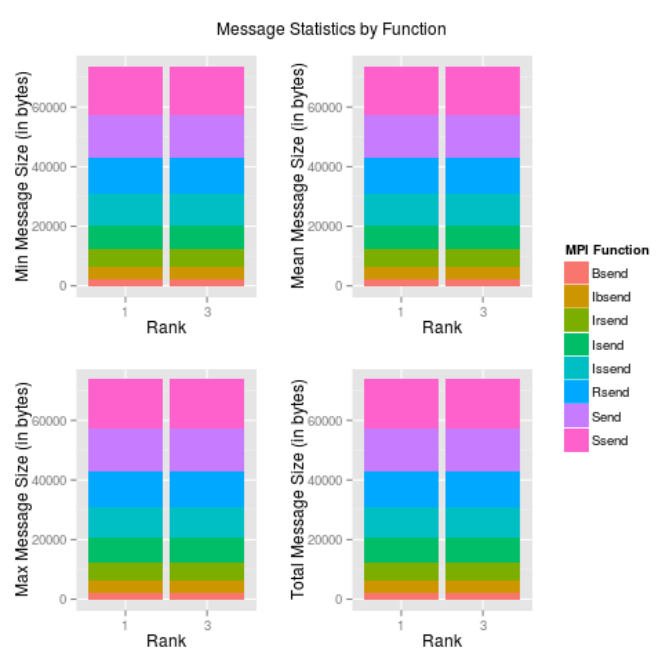
2. Run code

```
mpirun -np 64 Rscript
    my_script.R
```

3. Analyze results

```
library(pbdPROF)
prof <- read.prof(
    "profiler_output.mpiP")
plot(prof)
```

Publication-quality graphs



pbdR Paradigms

pbdR programs are R programs!

Differences:

- Batch execution (non-interactive).
- Parallel code utilizes Single Program/Multiple Data (SPMD) style
- Emphasizes data parallelism.

Batch Execution

- Running a serial R program in batch:

```
Rscript my_script.r
```

or

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

- Running a parallel (with MPI) R program in batch:

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

Single Program/Multiple Data (SPMD)

- SPMD is a programming *paradigm*.
- Not to be confused with SIMD.

Paradigms

Programming models
e.g. Procedural, OOP, Functional, SPMD, ...

SIMD

Hardware instructions
e.g. MMX, SSE, ...

SPMD is arguably the simplest extension of serial programming.

Single Program/Multiple Data (SPMD)

- 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.

Contents

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

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

Quick Example 1

Rank Query: 1_rank.r

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

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

finalize()
```

Execute this script via:

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

Sample Output:

```
COMM.RANK = 0
[1] 0
COMM.RANK = 1
[1] 1
```

Quick Example 2

Hello World: 2_hello.r

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

comm.print("Hello, world")

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

finalize()
```

Execute this script via:

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

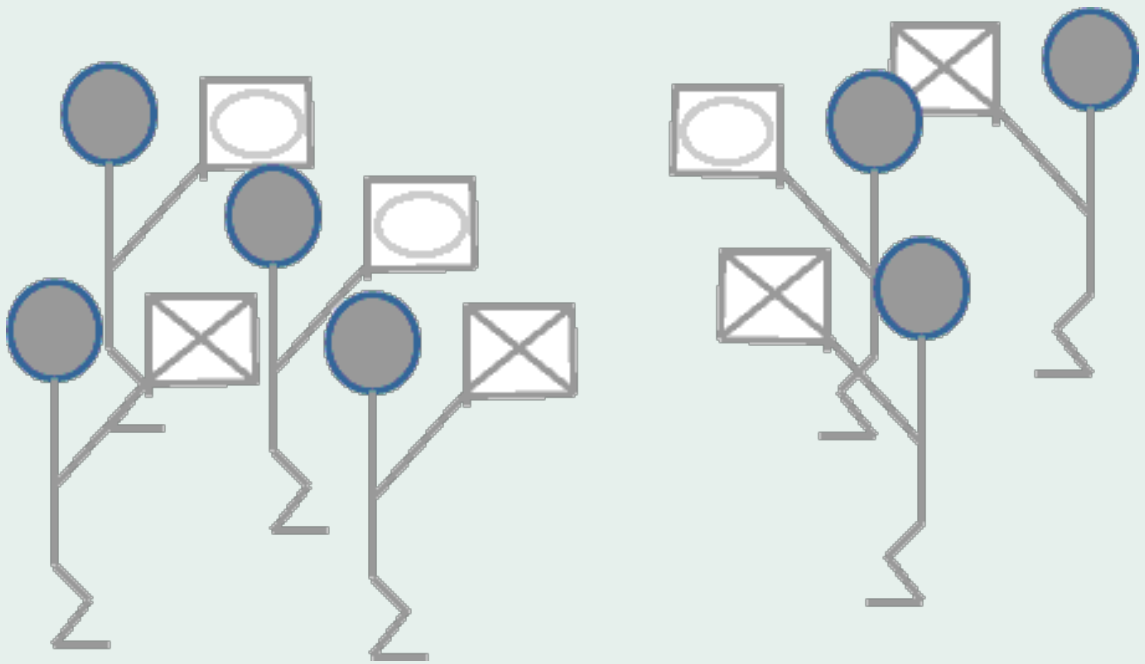
Sample Output:

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

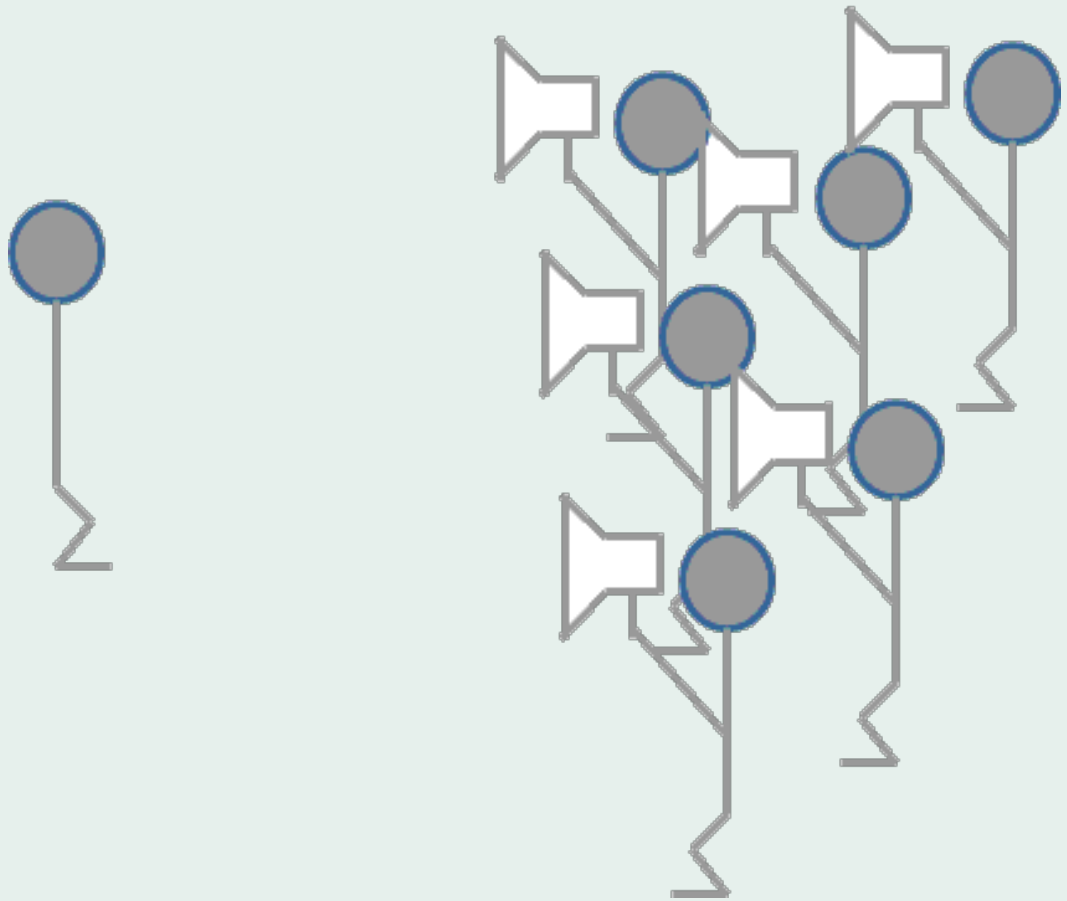
MPI Operations

1. Reduce
2. Gather
3. Broadcast
4. Barrier

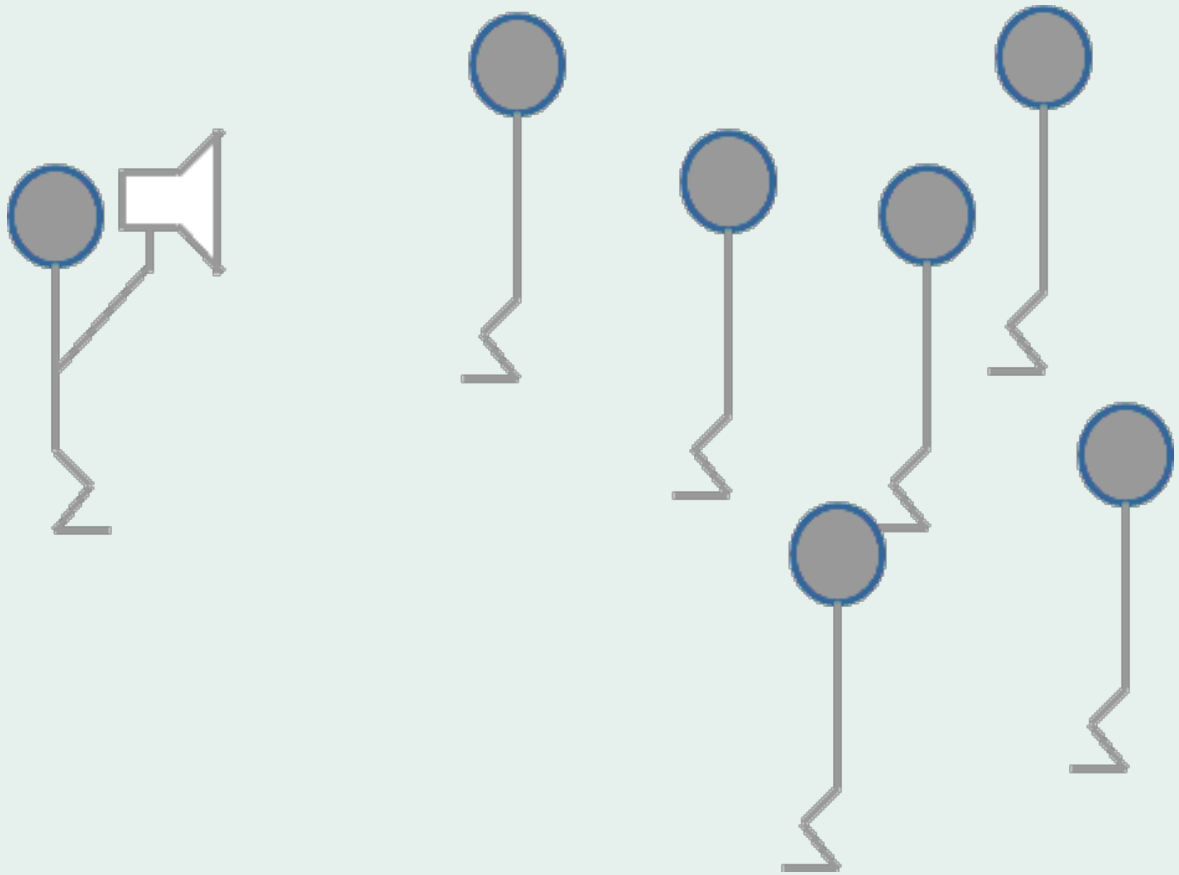
Reductions — Combine results into single result



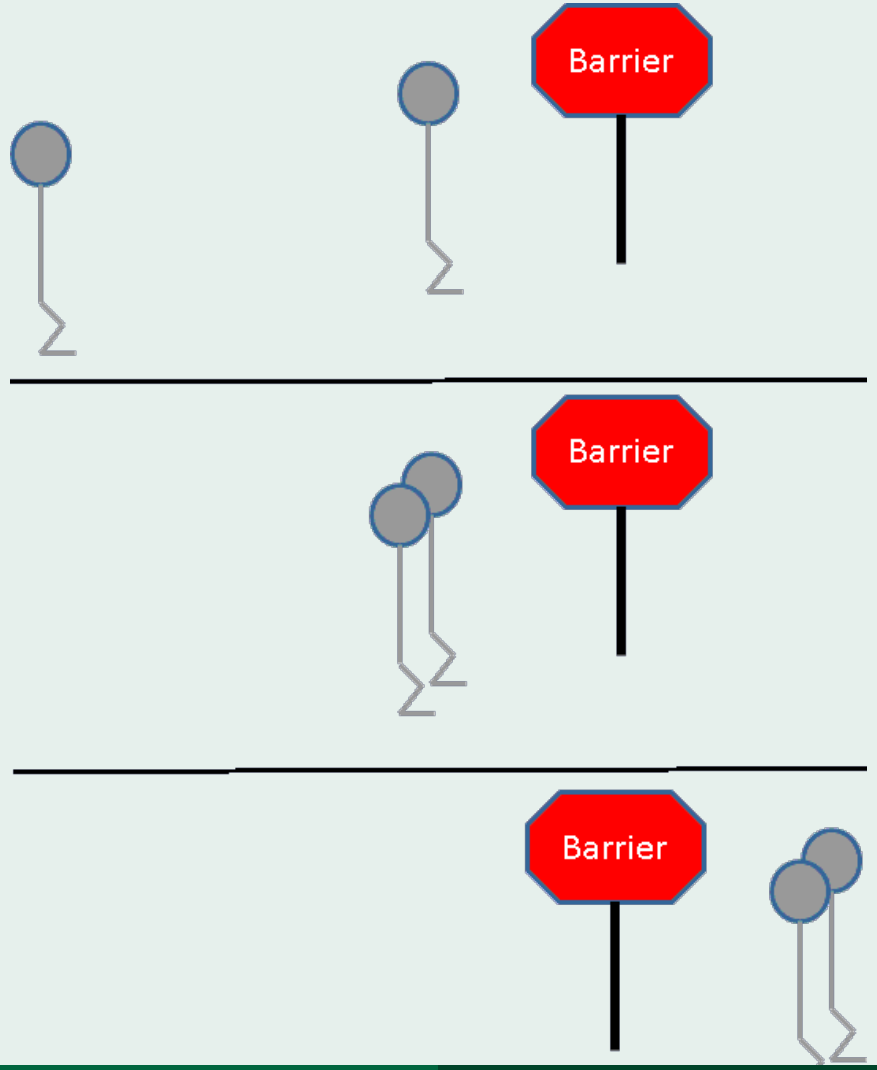
Gather — Many-to-one



Broadcast — One-to-many



Barrier — Synchronization



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, quietly=TRUE)
init()

comm.set.seed(diff=TRUE)

n <- sample(1:10, size=1)

gt <- gather(n)
comm.print(unlist(gt))

sm <- allreduce(n, op='sum')
comm.print(sm, all.rank=T)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 3_gt.r
```

Sample Output:

```
COMM.RANK = 0
[1] 2 8
COMM.RANK = 0
[1] 10
COMM.RANK = 1
[1] 10
```

Quick Example 4

Broadcast: 4_bcast.r

```
library(pbdMPI, quietly=T)
init()

if (comm.rank()==0){
  x <- matrix(1:4, nrow=2)
} else {
  x <- NULL
}

y <- bcast(x, rank.source=0)

comm.print(y, rank=1)

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
```

MPI Package Controls

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

Other pbdMPI Tools

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"))
  }
  barrier()
}

comm.cat("\n")

comm.cat(paste("Hello", comm.rank()+1, "of",
    comm.size(), "\n"), all.rank=TRUE)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 5_barrier.r
```

Sample Output:

```
Hello 1 of 2
Hello 2 of 2
```

Random Seeds

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).

Other pbdMPI Tools

Quick Example 6

Timing: 6_timer.r

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

comm.set.seed(diff=T)

test <- function(timed)
{
  ltime <- system.time(timed)[3]

  mintime <- allreduce(ltime, op='min')
  maxtime <- allreduce(ltime, op='max')
  meantime <- allreduce(ltime, op='sum')/comm.size()

  return(data.frame(min=mintime, mean=meantime,
      max=maxtime))
}

times <- test(rnorm(1e6)) # ~7.6MiB of data
comm.print(times)

finalize()
```

Execute this script via:

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

Sample Output:

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

Other Helper Tools

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()`

Quick Comments for Using pbdMPI

1. Start by loading the package:

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

2. Always initialize before starting and finalize when finished:

```
init()

# ...

finalize()
```

Contents

4 The Generalized Block Distribution
- The GBD Data Structure
- Example GBD Distributions

Distributing Data

Problem: How to distribute the data

$$x = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ x_{9,1} & x_{9,2} & x_{9,3} \\ x_{10,1} & x_{10,2} & x_{10,3} \end{bmatrix}_{10\times 3}$$

?

Distributing a Matrix Across 4 Processors: Block Distribution

Data

$$x = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ \hline x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ \hline x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ x_{9,1} & x_{9,2} & x_{9,3} \\ \hline x_{10,1} & x_{10,2} & x_{10,3} \end{bmatrix}_{10\times 3}$$

Processors

0
1
2
3

Distributing a Matrix Across 4 Processors: Local Load Balance

Data

$$x = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ \hline x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ \hline x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ \hline x_{9,1} & x_{9,2} & x_{9,3} \\ x_{10,1} & x_{10,2} & x_{10,3} \end{bmatrix}_{10\times 3}$$

Processors

0
1
2
3

The GBD Data Structure

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

1. 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*.
5. GBD is often *locally balanced*, where each processor owns (almost) the same amount of data. But this is not required.

$$\left[\begin{array}{ccc} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ \hline x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ \hline x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ \hline x_{9,1} & x_{9,2} & x_{9,3} \\ x_{10,1} & x_{10,2} & x_{10,3} \end{array}\right]$$

6. 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.
7. GBD is (relatively) easy to understand, but can lead to bottlenecks if you have many more columns than rows.

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.

Understanding GBD: Global Matrix

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{9\times 9}$$

Processors = 0 1 2 3 4 5

Understanding GBD: Load Balanced GBD

$$x = \left[\begin{array}{ccccccccc} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ \hline x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

Processors = 0 1 2 3 4 5

Understanding GBD: Local View

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \end{bmatrix}_{2\times 9}$$

$$\begin{bmatrix} x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \end{bmatrix}_{2\times 9}$$

$$\begin{bmatrix} x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \end{bmatrix}_{2\times 9}$$

$$\begin{bmatrix} x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \end{bmatrix}_{1\times 9}$$

$$\begin{bmatrix} x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \end{bmatrix}_{1\times 9}$$

$$\begin{bmatrix} x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{1\times 9}$$

Processors = 0 1 2 3 4 5

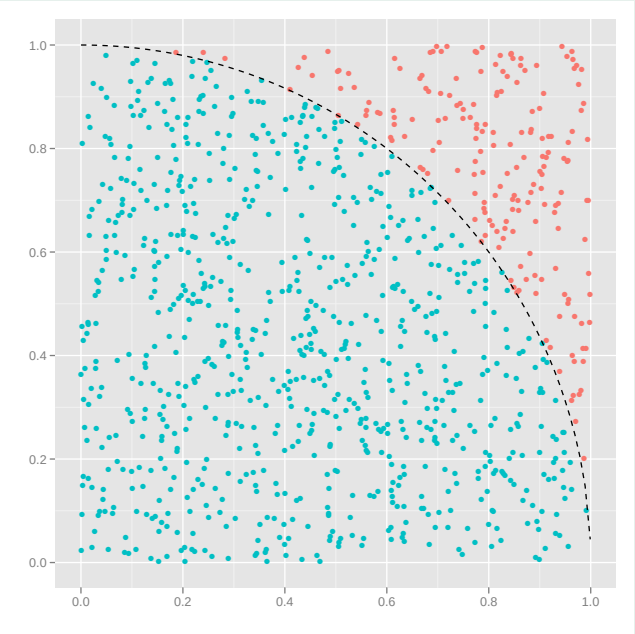
Contents

5 Basic Statistics Examples
- pbdMPI Example: Monte Carlo Simulation
- pbdMPI Example: Sample Covariance
- pbdMPI Example: Linear Regression

Example 1: Monte Carlo Simulation

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

$$\pi \approx 4\left(\frac{\#\ Inside\ Circle}{\#\ Total}\right) = 4\left(\frac{\#\ \text{Blue}}{\#\ \text{Blue} + \#\ \text{Red}}\right)$$



Example 1: Monte Carlo Simulation GBD Algorithm

1. 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 $x^2 + y^2 \leq 1$
4. Ask everyone else what their answer is; sum it all up.
5. Take this new answer, multiply by 4 and divide by n
6. If my rank is 0, print the result.

Example 1: Monte Carlo Simulation Code

Serial Code

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

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)

finalize()
```

pbdMPI Example: Monte Carlo Simulation

Note

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

Example 2: Sample Covariance

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

Example 2: Sample Covariance GBD Algorithm

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

Example 2: Sample Covariance Code

Serial Code

```
N <- nrow(X)
mu <- colSums(X) / N

X <- sweep(X, STATS=mu, MARGIN=2)
Cov.X <- crossprod(X) / (N-1)

print(Cov.X)
```

Parallel Code

```
N <- allreduce(nrow(X.gbd), op="sum")
mu <- allreduce(colSums(X.gbd) / N, op="sum")

X.gbd <- sweep(X.gbd, STATS=mu, MARGIN=2)
Cov.X <- allreduce(crossprod(X.gbd), op="sum") / (N-1)

comm.print(Cov.X)
```

Example 3: Linear Regression

Find $\boldsymbol{\beta}$ such that

$$y = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

When X is full rank,

$$\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T y$$

Example 3: Linear Regression GBD Algorithm

1. 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.
4. Locally, compute $A^{-1} * B$

Example 3: Linear Regression Code

Serial Code

```
tX <- t(X)
A <- tX %*% X
B <- tX %*% y

ols <- solve(A) %*% B
```

Parallel Code

```
tX.gbd <- t(X.gbd)
A <- allreduce(tX.gbd %*% X.gbd, op = "sum")
B <- allreduce(tX.gbd %*% y.gbd, op = "sum")

ols <- solve(A) %*% B
```

Contents

6 Data Input
- Serial Data Input
- Parallel Data Input

Separate manual: http://r-project.org/

- scan()
- read.table()
- read.csv()
- socket

CSV Data: Read Serial then Distribute

Listing:

```
library(pbdDMAT)
if(comm.rank() == 0) { # only read on process 0
  x <- read.csv("myfile.csv")
} else {
  x <- NULL
}

dx <- as.ddmatrix(x)
```

New Issues

- How to read in parallel?
- CSV, SQL, NetCDF4, HDF, ADIOS, custom binary
- How to partition data across nodes?
- How to structure for scalable libraries?
- Read directly into form needed or restructure?
- ...
- A lot of work needed here!

CSV Data

Serial Code

```
d <- read.csv(``x.csv'')
```

Parallel Code 0_readcsv.r

```
library(pbdDEMO, quiet = TRUE)
init.grid()
dx <- read.csv.ddmatrix("x.csv", header=TRUE,
          sep='','', nrows=10, ncols=10,
          num.rdrs=2, ICTXT=0)
comm.print(dx)
finalize()
```

CSV Data

NetCDF4 Files

```
### Must determine who will read what portion(s) and how to assemble
them before reading

### parallel read after determining st and co
nc <- nc_open_par(file.name)

nc_var_par_access(nc, "TREFHT")
new.X.gbdc <- ncvar_get(nc, "TREFHT", start = st, count = co)
nc_close(nc)

finalize()
```

Parallel Data Input

CSV Data

3d Block Binary Reader

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

## Raw data dimensions in file
data.dim <- c(2048, 2048, 2048)

## global subcube definition
g.start <- c(1, 1, 513)
g.dim <- c(64, 64, 1024)

## local dimension and start
my.dim <- g.dim / c(1, 1, comm.size())
my.start <- g.start + c(0, 0, comm.rank()*my.dim[3])

size <- 4 # file is single precision floats
project <- "/lustre/atlas/proj-shared/stf006/d7r/inv_cascade"
filex <- paste(project, "rot_abc_2048_kf50/outs/vx.061.out", sep="/")

vx <- block3d.read(filex, data.dim, my.start, my.dim, size)

save.file <- paste("xyz.RData", comm.rank(), sep="")
save(vx, file=save.file)

## make a ddmatrix from local data
## reshape 3d array into a matrix for PCA (EOF) computation
## first two dimensions become rows and third becomes columns

## local reshape dimensions
my.nrow <- prod(my.dim[1:2])
my.ncol <- my.dim[3]
ldim <- c(my.nrow, my.ncol)

## global reshape dimensions
g.nrow <- prod(g.dim[1:2])
g.ncol <- g.dim[3]
gdim <- c(g.nrow, g.ncol)

## now reshape local
X <- matrix(vx, nrow=my.nrow, ncol=my.ncol, byrow=FALSE)

## glue local pieces into a ddmatrix
X <- new("ddmatrix", Data=X, dim=gdim, ldim=ldim, bldim=ldim, ICTXT=1)

## transform to 2d block cyclic
X <- redistribute(X, bldim=c(8,8), ICTXT=0)
```

Parallel Data Input

CSV Data

3d Block Binary Reader

```
block3d.read <- function(file, data.dim, my.start, my.dim, size=4) {
    con.x <- file(file, "rb", blocking=TRUE)
    if(isSeekable(con.x)) {

        start <- sum((my.start - 1) * c(1, cumprod(data.dim)[-length(data.dim)]))

        x <- rep(NA, prod(my.dim))

        block <- 1:my.dim[1]

        for(j in 1:my.dim[3]) {
            sofar <- 0
            for(i in 1:my.dim[2]) {
                seek(con.x, where=start, rw="read", origin="start")
                x[block] <- readBin(con=con.x, what="numeric",
                                    n=my.dim[1], size=size)
                block <- block + my.dim[1]

                start <- start + data.dim[1]*size
                sofar <- sofar + data.dim[1]*size
            }
            start <- start - sofar + data.dim[1]*data.dim[2]*size
        }
    }
  else {
      x <- NULL
      comm.print(paste("Sorry ...", file, "not seakable!"))
  }
    close(con.x)
    x
}
```

Contents

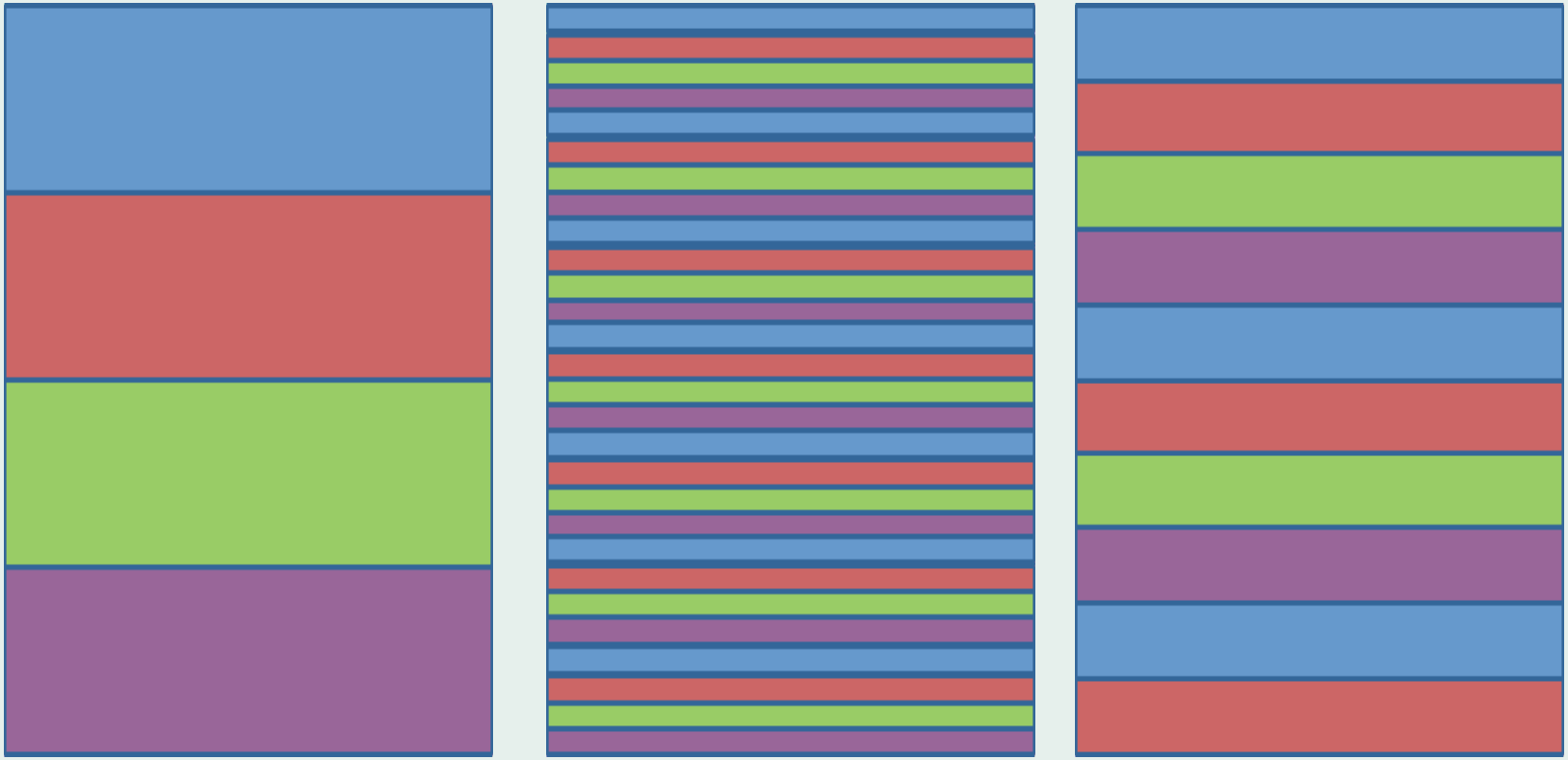
7 Introduction to pbdDMAT and the ddmatrix Structure
- Introduction to Distributed Matrices
- `ddmatrix`Distributions
- pbdDMAT

Distributed Matrices

Most problems in data science are matrix algebra problems, so:

$$\text{Distributed matrices} \implies \text{Handle Bigger data}$$

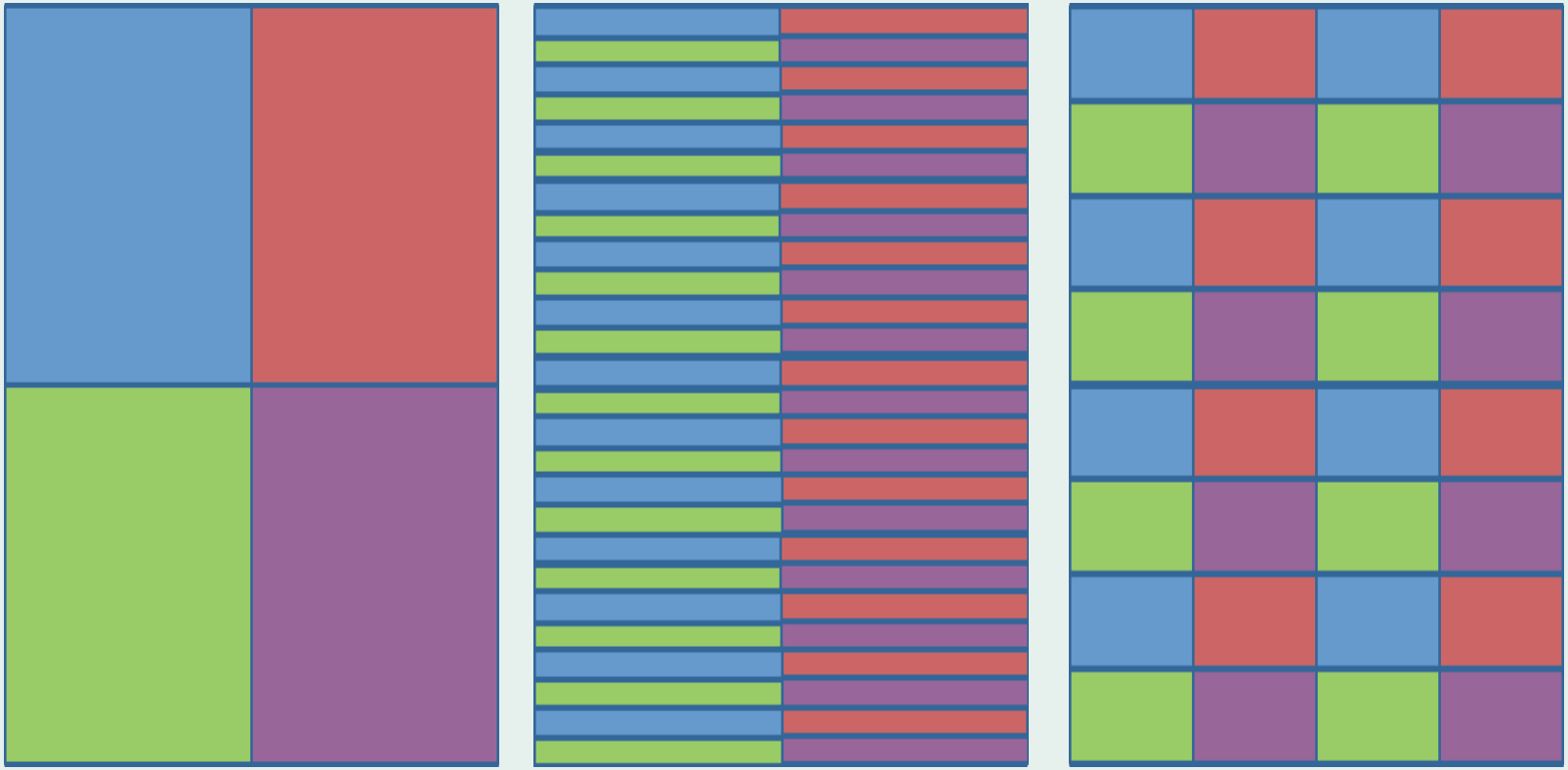
Distributed Matrices



(a) Block (b) Cyclic (c) Block-Cyclic

Figure: Matrix Distribution Schemes

Distributed Matrices



(a) 2d Block (b) 2d Cyclic (c) 2d Block-Cyclic

Figure: Matrix Distribution Schemes Onto a 2-Dimensional Grid

Processor Grid Shapes

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

Table: Processor Grid Shapes with 6 Processors

Understanding ddmatrix: Global Matrix

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{9\times 9}$$

ddmatrix: 1-dimensional Row Block

$$x = \left[\begin{array}{ccccccccc} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ \hline x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \left|\begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \end{array}\right| = \left|\begin{array}{c} (0,0) \\ (1,0) \\ (2,0) \\ (3,0) \end{array}\right|$$

ddmatrix: 2-dimensional Row Block

$$x = \left[\begin{array}{ccccc|cccc} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ \hline x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

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

ddmatrix: 1-dimensional Row Cyclic

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{9\times 9}$$

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

ddmatrix: 2-dimensional Row Cyclic

$$x = \left[\begin{array}{ccccc|cccc} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ \hline x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ \hline x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ \hline x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ \hline x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

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

ddmatrix: 2-dimensional Block-Cyclic

$$x = \left[\begin{array}{cc|cc|cc|cc|c} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

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

The ddmatrix Data Structure

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

ddmatrix: 2-dimensional Block-Cyclic with 6 Processors

$$x = \left[\begin{array}{cc|cc|cc|cc|c} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

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

Understanding `ddmatrix`: Local View

$$\left[\begin{array}{cc|cc} x_{11} & x_{12} & x_{17} & x_{18} \\ x_{21} & x_{22} & x_{27} & x_{28} \\ \hline x_{51} & x_{52} & x_{57} & x_{58} \\ x_{61} & x_{62} & x_{67} & x_{68} \\ \hline x_{91} & x_{92} & x_{97} & x_{98} \end{array}\right]_{5\times 4} \left[\begin{array}{cc|c} x_{13} & x_{14} & x_{19} \\ x_{23} & x_{24} & x_{29} \\ \hline x_{53} & x_{54} & x_{59} \\ x_{63} & x_{64} & x_{69} \\ \hline x_{93} & x_{94} & x_{99} \end{array}\right]_{5\times 3} \left[\begin{array}{cc} x_{15} & x_{16} \\ x_{25} & x_{26} \\ \hline x_{55} & x_{56} \\ x_{65} & x_{66} \\ \hline x_{95} & x_{96} \end{array}\right]_{5\times 2}$$

$$\left[\begin{array}{cc|cc} x_{31} & x_{32} & x_{37} & x_{38} \\ x_{41} & x_{42} & x_{47} & x_{48} \\ \hline x_{71} & x_{72} & x_{77} & x_{78} \\ x_{81} & x_{82} & x_{87} & x_{88} \end{array}\right]_{4\times 4} \left[\begin{array}{cc|c} x_{33} & x_{34} & x_{39} \\ x_{43} & x_{44} & x_{49} \\ \hline x_{73} & x_{74} & x_{79} \\ x_{83} & x_{84} & x_{89} \end{array}\right]_{4\times 3} \left[\begin{array}{cc} x_{35} & x_{36} \\ x_{45} & x_{46} \\ \hline x_{75} & x_{76} \\ x_{85} & x_{86} \end{array}\right]_{4\times 2}$$

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

The ddmatrix Data Structure

1. ddmatrix is *distributed*. No one processor owns all of the matrix.
2. ddmatrix is *non-overlapping*. Any piece owned by one processor is owned by no other processors.
3. ddmatrix can be row-contiguous or not, depending on the processor grid and blocking factor used.
4. ddmatrix is locally column-major and globally, it depends. . .

$$\left[\begin{array}{cc|cc|c} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} \\ \hline x_{31} & x_{32} & x_{33} & x_{34} & x_{35} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} \\ \hline x_{51} & x_{52} & x_{53} & x_{54} & x_{55} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} \\ \hline x_{91} & x_{92} & x_{93} & x_{94} & x_{95} \end{array}\right]$$

6. GBD is a generalization of the one-dimensional block ddmatrix distribution. Otherwise there is no relation.
7. ddmatrix is confusing, but very robust.

Pros and Cons of This Data Structure

Pros

- Robust for matrix computations.

Cons

- Confusing layout.

This is why we hide most of the distributed details.

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

Methods for class `ddmatrix`

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

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

Serial Code

```
cov(x)
```

Parallel Code

```
cov(x)
```

Comparing pbdMPI and pbdDMAT

pbdMPI:

- MPI + sugar.
- `GBD` not the only structure **pbdMPI** can handle (just a useful convention).

pbdDMAT:

- More of a software package.
- The `ddmatrix` structure *must* be used for **pbdDMAT**.
- If the data is not 2d block-cyclic compatible, `ddmatrix` will *definitely* give the wrong answer.

Quick Comments for Using pbdDMAT

1. Start by loading the package:

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

2. Always initialize before starting and finalize when finished:

```
init.grid()

# ...

finalize()
```

3. Distributed `ddmatrix` objects will be given the suffix `.dmat` to visually help distinguish them from global objects. This suffix carries no semantic meaning.

Contents

8 Examples Using pbdDMAT
- Manipulating `ddmatrix`Objects
- Statistics Examples with pbdDMAT
- RandSVD

Manipulating ddmatrix Objects

Example 1: ddmatrix Construction

Generate a global matrix and distribute it

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

# Common global on all processors --> distributed
x <- matrix(1:100, nrow=10, ncol=10)
x.dmat <- as.ddmatrix(x)

x.dmat

# Global on processor 0 --> distributed
if (comm.rank()==0){
  y <- matrix(1:100, nrow=10, ncol=10)
} else {
  y <- NULL
}
y.dmat <- as.ddmatrix(y)

y.dmat

finalize()
```

Execute this script via:

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

Example 2: ddmatrix Construction

Generate locally only what is needed

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

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

id.dmat <- diag(1, nrow=100, ncol=100, type="ddmatrix")
id.dmat

comm.set.seed(diff=T)
rand.dmat <- ddmatrix("rnorm", nrow=100, ncol=100,
    mean=10, sd=100)
rand.dmat

finalize()
```

Execute this script via:

Example 3: ddmatrix Operations

Generate locally only what is needed

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

x.dmat <- ddmatrix(1:30, nrow=10)
y.dmat <- x.dmat[c(1, 3, 5, 7, 9), -3]

comm.print(y.dmat)
y <- as.matrix(y.dmat)
comm.print(y)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 3_extract.r
```

Example 4: More ddmatrix Operations

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

x.dmat <- ddmatrix(1:30, nrow=10)
y.dmat <- x.dmat + 1:7
z.dmat <- scale(x.dmat, center=TRUE, scale=TRUE)

y <- as.matrix(y.dmat)
z <- as.matrix(z.dmat)

comm.print(y)
comm.print(z)

finalize()
```

Execute this script via:

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

Sample Covariance

Serial Code

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

Parallel Code

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

Linear Regression

Serial Code

```
tX <- t(X)
A <- tX %*% X
B <- tX %*% y

ols <- solve(A) %*% B

# or
ols <- lm.fit(X, y)
```

Parallel Code

```
tX <- t(X)
A <- tX %*% X
B <- tX %*% y

ols <- solve(A) %*% B

# or
ols <- lm.fit(X, y)
```

Example 5: PCA

PCA: pca.r

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

n <- 1e4
p <- 250

comm.set.seed(diff=T)
x.dmat <- ddmatrix("rnorm", nrow=n, ncol=p, mean=100, sd=25)

pca <- prcomp(x=x.dmat, retx=TRUE, scale=TRUE)
prop_var <- cumsum(pca$sdev)/sum(pca$sdev)
i <- max(min(which(prop_var > 0.9)) - 1, 1)

y.dmat <- pca$x[, 1:i]

comm.cat("\nCols: ", i, "\n", quiet=T)
comm.cat("%Cols:", i/dim(x.dmat)[2], "\n\n", quiet=T)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 5_pca.r
```

Sample Output:

```
Cols:  221
%Cols: 0.884
```

Distributed Matrices

pbdDEMO contains many other examples of reading and managing GBD and `ddmatrix` data

Randomized SVD[1]

Prototype for Randomized SVD

Given an $m \times n$ matrix $\boldsymbol{A}$, a target number k of singular vectors, and an exponent q (say, $q = 1$ or $q = 2$), this procedure computes an approximate rank-$2k$ factorization $\boldsymbol{U\Sigma V}^*$, where $\boldsymbol{U}$ and $\boldsymbol{V}$ are orthonormal, and $\boldsymbol{\Sigma}$ is nonnegative and diagonal.

Stage A:

1. Generate an $n \times 2k$ Gaussian test matrix $\boldsymbol{\Omega}$.
2. Form $\boldsymbol{Y} = (\boldsymbol{AA}^*)^q \boldsymbol{A\Omega}$ by multiplying alternately with $\boldsymbol{A}$ and $\boldsymbol{A}^*$.
3. Construct a matrix $\boldsymbol{Q}$ whose columns form an orthonormal basis for the range of $\boldsymbol{Y}$.

Stage B:

4. Form $\boldsymbol{B} = \boldsymbol{Q}^*\boldsymbol{A}$.
5. Compute an SVD of the small matrix: $\boldsymbol{B} = \widetilde{\boldsymbol{U}}\boldsymbol{\Sigma V}^*$.
6. Set $\boldsymbol{U} = \boldsymbol{Q}\widetilde{\boldsymbol{U}}$.

Note: The computation of $\boldsymbol{Y}$ in step 2 is vulnerable to round-off errors. When high accuracy is required, we must incorporate an orthonormalization step between each application of $\boldsymbol{A}$ and $\boldsymbol{A}^*$; see Algorithm 4.4.

Algorithm 4.4: Randomized Subspace Iteration

Given an $m \times n$ matrix $\boldsymbol{A}$ and integers ℓ and q, this algorithm computes an $m \times \ell$ orthonormal matrix $\boldsymbol{Q}$ whose range approximates the range of $\boldsymbol{A}$.

1. Draw an $n \times \ell$ standard Gaussian matrix $\boldsymbol{\Omega}$.
2. Form $\boldsymbol{Y}_0 = \boldsymbol{A\Omega}$ and compute its QR factorization $\boldsymbol{Y}_0 = \boldsymbol{Q}_0\boldsymbol{R}_0$.
3. **for** $j = 1, 2, \ldots, q$
4. Form $\widetilde{\boldsymbol{Y}}_j = \boldsymbol{A}^*\boldsymbol{Q}_{j-1}$ and compute its QR factorization $\widetilde{\boldsymbol{Y}}_j = \widetilde{\boldsymbol{Q}}_j\widetilde{\boldsymbol{R}}_j$.
5. Form $\boldsymbol{Y}_j = \boldsymbol{A}\widetilde{\boldsymbol{Q}}_j$ and compute its QR factorization $\boldsymbol{Y}_j = \boldsymbol{Q}_j\boldsymbol{R}_j$.
6. **end**
7. $\boldsymbol{Q} = \boldsymbol{Q}_q$.

Serial R

```
randSVD <- function(A, k, q=3)
  {
    ## Stage A
    Omega <- matrix(rnorm(n*2*k),
                    nrow=n, ncol=2*k)
    Y <- A %*% Omega
    Q <- qr.Q(qr(Y))
    At <- t(A)
    for(i in 1:q)
      {
        Y <- At %*% Q
        Q <- qr.Q(qr(Y))
        Y <- A %*% Q
        Q <- qr.Q(qr(Y))
      }

    ## Stage B
    B <- t(Q) %*% A
    U <- La.svd(B)$u
    U <- Q %*% U
    U[, 1:k]
  }
```

[1] Halko N, Martinsson P-G and Tropp J A 2011 Finding structure with randomness: probabilistic algorithms for

Randomized SVD

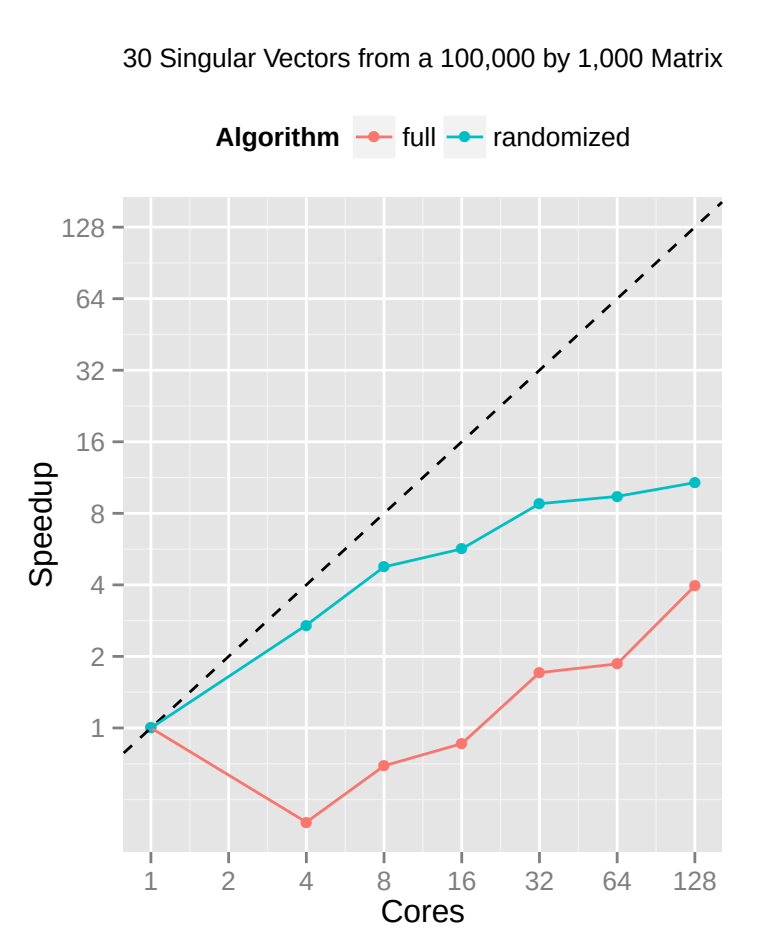
Serial R

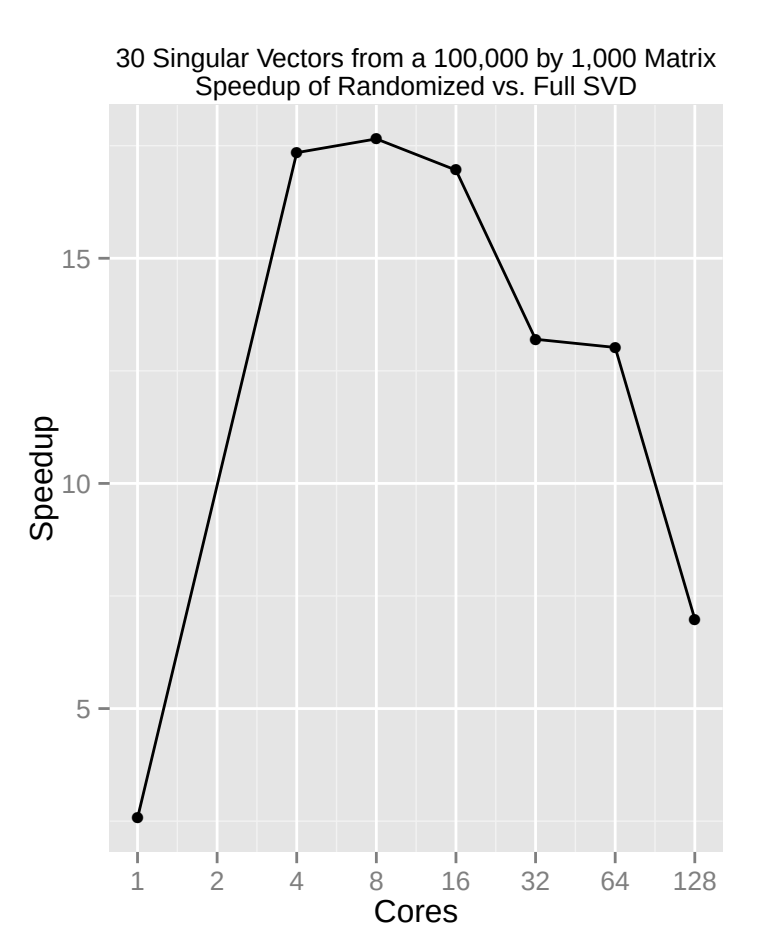
```
randSVD <- function(A, k, q=3)
  {
    ## Stage A
    Omega <- matrix(rnorm(n*2*k),
              nrow=n, ncol=2*k)
    Y <- A %*% Omega
    Q <- qr.Q(qr(Y))
    At <- t(A)
    for(i in 1:q)
      {
        Y <- At %*% Q
        Q <- qr.Q(qr(Y))
        Y <- A %*% Q
        Q <- qr.Q(qr(Y))
      }

    ## Stage B
    B <- t(Q) %*% A
    U <- La.svd(B)$u
    U <- Q %*% U
    U[, 1:k]
  }
```

Parallel pbdR

```
randSVD <- function(A, k, q=3)
  {
    ## Stage A
    Omega <- ddmatrix("rnorm",
              nrow=n, ncol=2*k)
    Y <- A %*% Omega
    Q <- qr.Q(qr(Y))
    At <- t(A)
    for(i in 1:q)
      {
        Y <- At %*% Q
        Q <- qr.Q(qr(Y))
        Y <- A %*% Q
        Q <- qr.Q(qr(Y))
      }

    ## Stage B
    B <- t(Q) %*% A
    U <- La.svd(B)$u
    U <- Q %*% U
    U[, 1:k]
  }
```

Randomized SVD





Contents

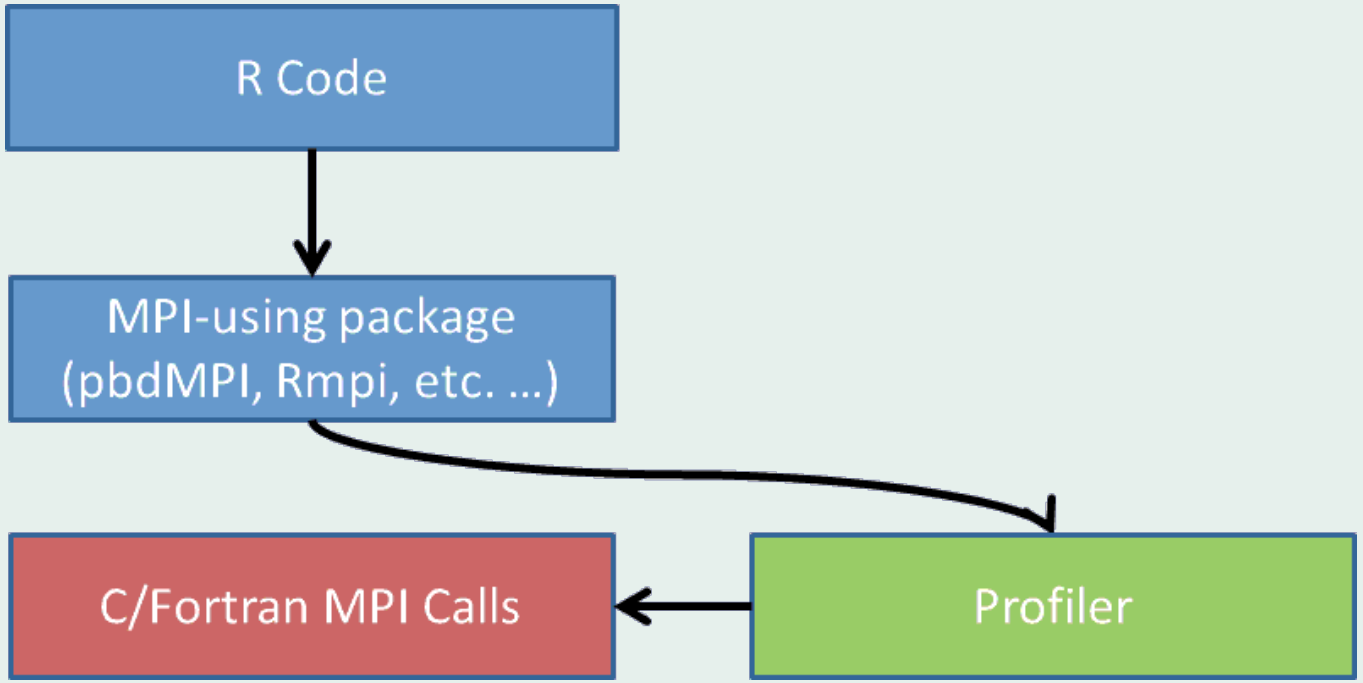
9 Profiling
- Profiling
- Installing pbdPROF
- Example

Introduction to **pbdPROF**

- Successful Google Summer of Code 2013 project.
- Available on the CRAN.
- Enables profiling of MPI-using R scripts.
- **pbdR** packages officially supported; can work with others...
- Also reads, parses, and plots profiler outputs.

How it works

MPI calls get hijacked by profiler and logged:



Introduction to **pbdPROF**

- Currently supports the profilers **fpmpi** and **mpiP**.
- **fpmpi** is distributed with **pbdPROF** and installs easily, but offers minimal profiling capabilities.
- **mpiP** is fully supported also, but harder to install.

Installing **pbdPROF**

1. Build **pbdPROF**.
2. Rebuild **pbdMPI** (linking with **pbdPROF**).
3. Run your analysis as usual.
4. Interactively analyze profiler outputs with **pbdPROF**.

Build **pbdPROF**

```
R CMD INSTALL pbdPROF_0.2-1.tar.gz
```

- The above installs **fpmpi**.
- **mpiP** can be used if you have a system installation available.
- See package vignette for more details and troubleshooting.

Rebuild **pbdMPI**

```
R CMD INSTALL pbdMPI_0.2-2.tar.gz
    --configure-args="--enable-pbdPROF"
```

- Any package which explicitly links with an MPI library must be rebuilt in this way (**pbdMPI**, **Rmpi**, ...).
- Other **pbdR** packages link with **pbdMPI**, and so do not need to be rebuilt.
- See **pbdPROF** vignette if something goes wrong.

Example Script

my_svd.r

```
library(pbdMPI, lib.loc="~/R/prof", quietly=TRUE)
library(pbdDMAT, quietly=T)
init.grid()

n <- 1000
x <- ddmatrix("rnorm", n, n)

asdf <- La.svd(x)


finalize()
```

Example Script

Run example with 4 ranks:

```
$ mpirun -np 4 Rscript my_svd.r
mpiP:
mpiP: mpiP: mpiP V3.3.0 (Build Sep 23 2013/14:00:47)
mpiP: Direct questions and errors to
    mpip-help@lists.sourceforge.net
mpiP:
Using 2x2 for the default grid size

mpiP:
mpiP: Storing mpiP output in [./R.4.5944.1.mpiP].
mpiP:
```

Read Profiler Data into R

Interactively (or in batch) Read in Profiler Data

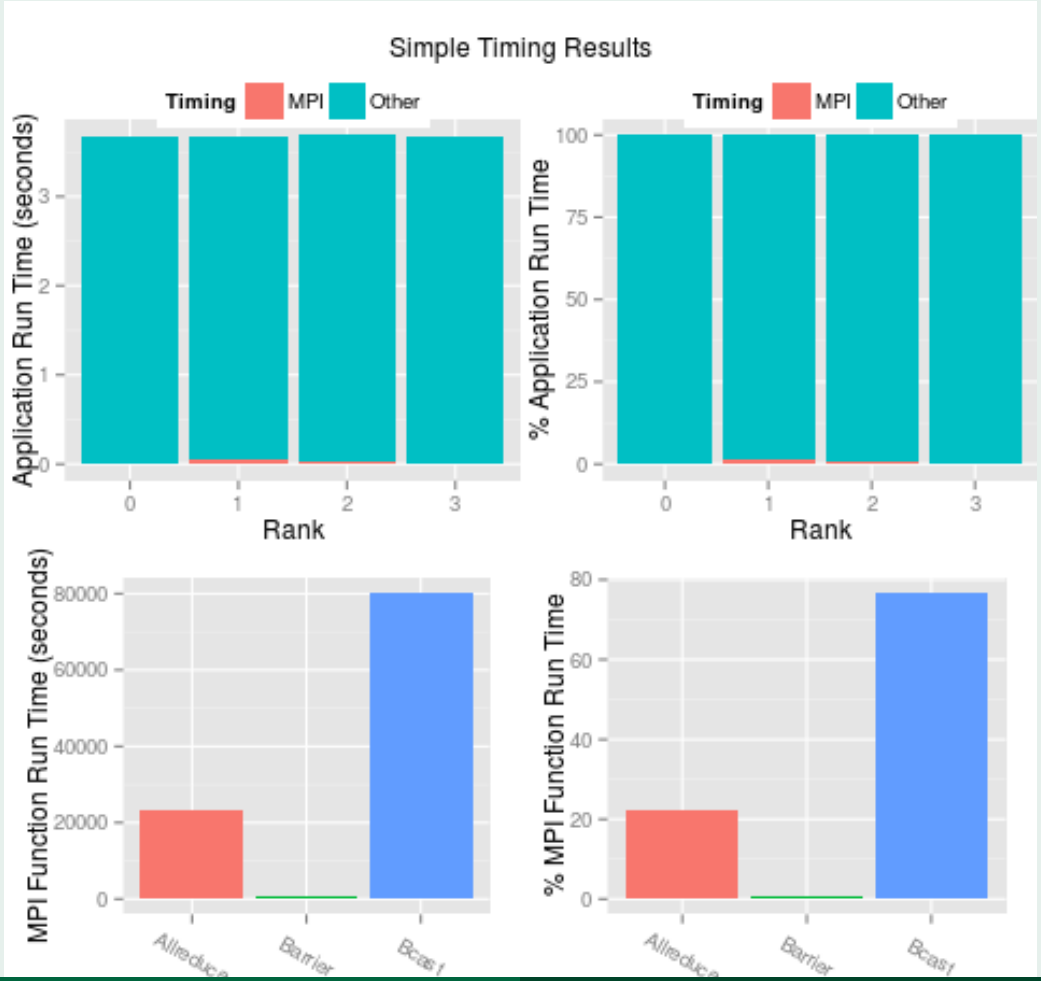
```
library(pbdPROF)
prof.data <- read.prof("R.4.28812.1.mpiP")
```

Partial Output of Example Data

```
> prof.data
An mpip profiler object:
[[1]]
  Task AppTime MPITime MPI.
1    0    5.71  0.0387 0.68
2    1    5.70  0.0297 0.52
3    2    5.71  0.0540 0.95
4    3    5.71  0.0355 0.62
5    *   22.80  0.1580 0.69

[[2]]
   ID Lev File.Address Line_Parent_Funct  MPI_Call
1   1   0 1.397301e+14         [unknown] Allreduce
2   2   0 1.397301e+14         [unknown]     Bcast
```

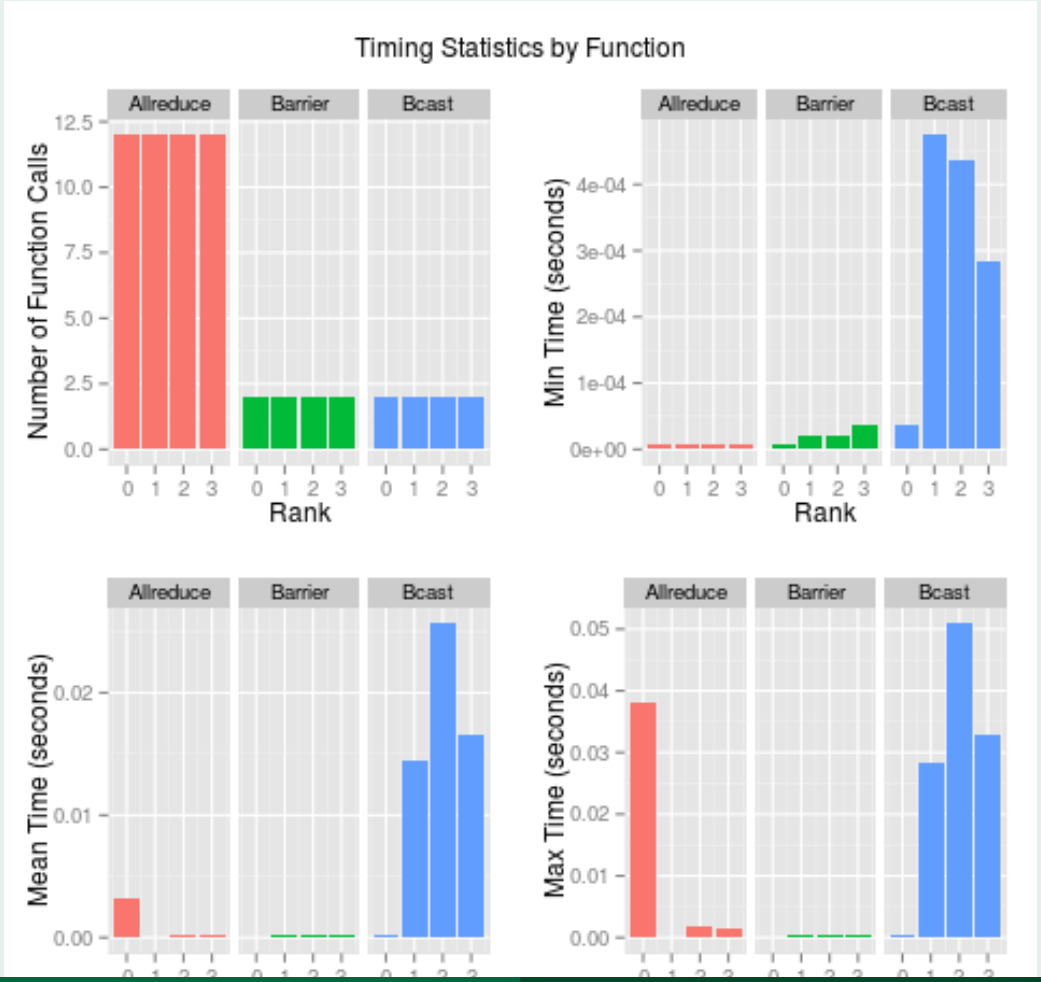
Generate plots

```
plot(prof.data)
```



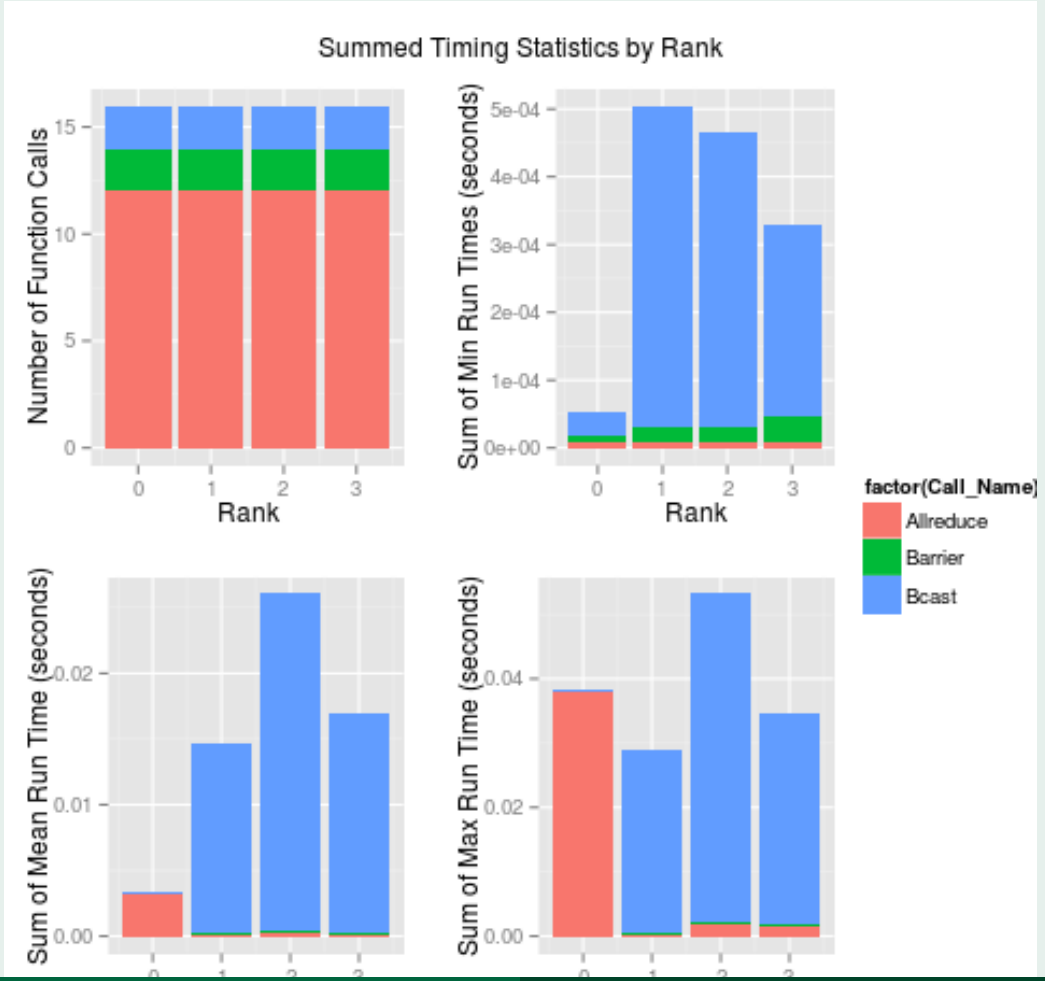
Generate plots

```
plot(prof.data, plot.type="stats1")
```



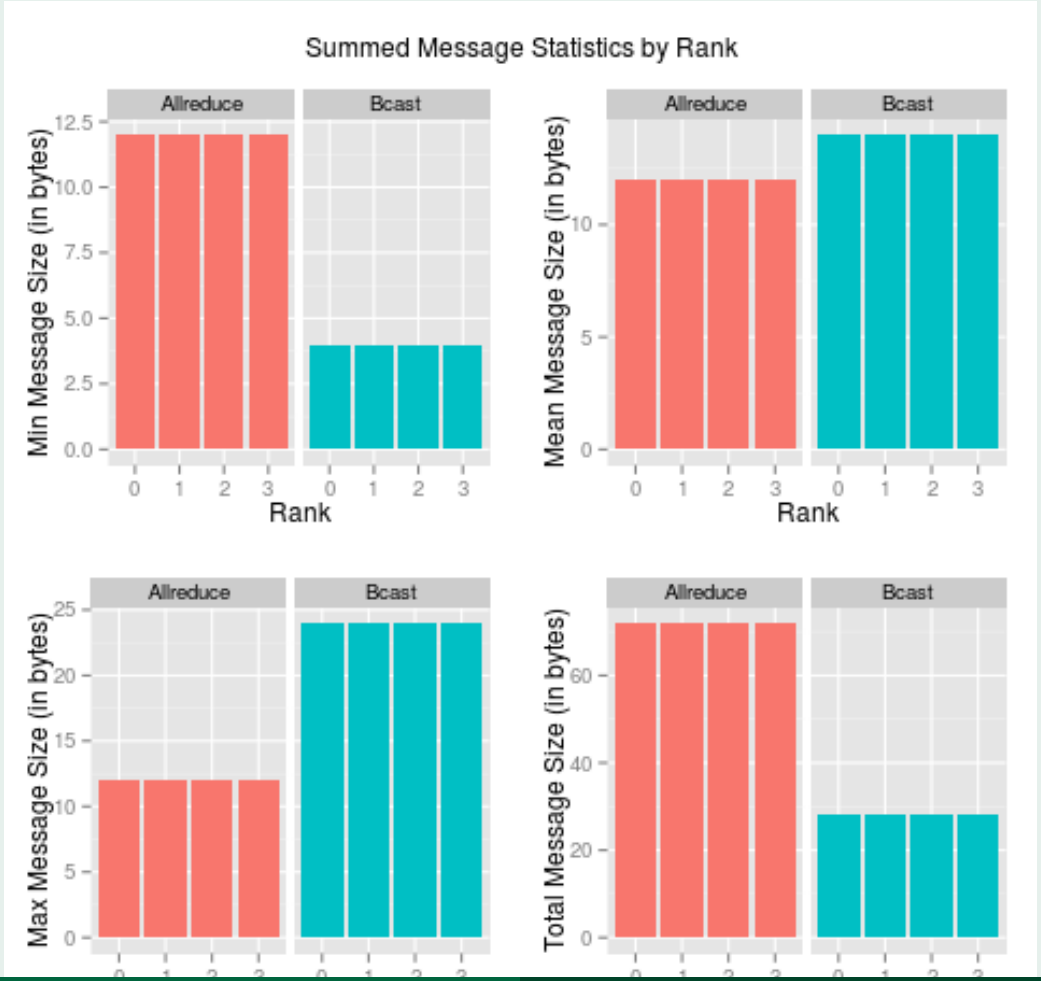
Generate plots

```
plot(prof.data, plot.type="stats2")
```



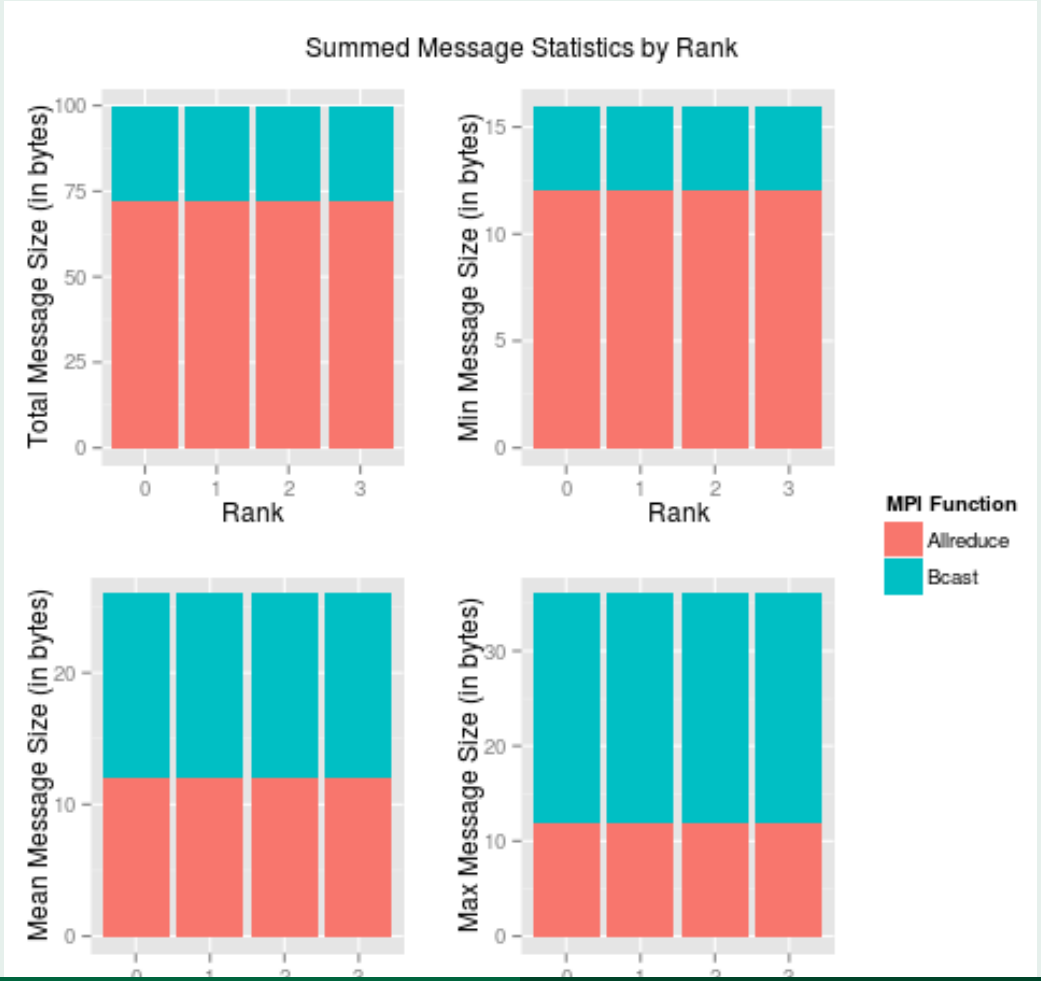
Generate plots

```
plot(prof.data, plot.type="messages1")
```



Generate plots

```
plot(prof.data, plot.type="messages2")
```



Contents

10 Example Applications
- Principal Components Analysis
- Parallel Plot Ensembles

Empirical Orthogonal Functions in Climate Analysis

- Computation and volume rendering of large-scale EOF coherent modes in rotating turbulent flow data, AGU Fall Meeting, December 2013

Principal Components Analysis

Coherent Modes in Turbulent Flow

Get and Redistribute the Data

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

## load local data (file assumes 4 processors!)
g.dim <- c(64, 64, 1024)
my.dim <- g.dim / c(1, 1, comm.size())
save.file <- paste("xyz.RData", comm.rank(), sep="") # assumes 4 processors!
load(save.file)

## reshape 3d array into a matrix for PCA (EOF) computation
## first two dimensions become rows and third becomes columns
## local reshape dimensions
my.nrow <- prod(my.dim[1:2])
my.ncol <- my.dim[3]
ldim <- c(my.nrow, my.ncol)

## global reshape dimensions
g.nrow <- prod(g.dim[1:2])
g.ncol <- g.dim[3]
gdim <- c(g.nrow, g.ncol)

## now reshape local
X <- matrix(vx, nrow=my.nrow, ncol=my.ncol, byrow=FALSE)
Y <- matrix(vy, nrow=my.nrow, ncol=my.ncol, byrow=FALSE)
Z <- matrix(vz, nrow=my.nrow, ncol=my.ncol, byrow=FALSE)

## glue local pieces into a ddmatrix
X <- new("ddmatrix", Data=X, dim=gdim, ldim=ldim, bldim=ldim, ICTXT=1)
Y <- new("ddmatrix", Data=Y, dim=gdim, ldim=ldim, bldim=ldim, ICTXT=1)
Z <- new("ddmatrix", Data=Z, dim=gdim, ldim=ldim, bldim=ldim, ICTXT=1)

## transform to 2d block cyclic
X <- redistribute(X, bldim=c(8,8), ICTXT=0)
Y <- redistribute(Y, bldim=c(8,8), ICTXT=0)
Z <- redistribute(Z, bldim=c(8,8), ICTXT=0)
```

Coherent Modes in Turbulent Flow

Compute PCA and do Scree Plot (0_pca.r)

```
E <- sqrt(X^2 + Y^2 + Z^2) # energy from velocity
E.pca <- prcomp(x=E, retx=TRUE, scale=FALSE)

# plot using one process
if(comm.rank() == 0)
  {
    ## scree plot for first 50 components
    variance <- E.pca$sdev^2  # note: all own sdev
    proportion <- variance[1:50]/sum(variance)
    cumulative <- cumsum(proportion)
    component <- 1:length(proportion)
    png("scree.png")
    plot(component, cumulative, ylim=c(0,1))
    points(component, proportion, type="h", col="blue")
    dev.off()
  }

finalize()
```

How can we plot in parallel?

- Several plots, one on each processor
- One plot by several processors

Parallel Plot Ensembles

Plots in parallel

png.slice

```
png.slice <- function(x, g.dim, lab="slice", title=lab,
    work.dir="", zero.center=TRUE, most.positive=TRUE)
{
  X <- array(as.vector(x), dim=g.dim)

  ## prepare zero centered topo.colors
  if(zero.center)
    {
       . . .
    }
  else
    zlim <- range(X)

  ## set most positive (for unique up to sign)
  if(most.positive)
    {
       . . .
    }

  ## make png file
  file <- paste(work.dir, lab, "-r", comm.rank(),
      ".png", sep="")
  png(file)
  image(x=1:g.dim[1], y=1:g.dim[2], z=X,
      col=topo.colors(40), useRaster=TRUE, asp=1,
      xlim=c(1, g.dim[1] + 1), ylim=c(1, g.dim[2] + 1),
      zlim=zlim)
  title(title)
  ret <- dev.off()
  invisible(ret)
}
```

Parallel Plot Ensembles

Plots in parallel

Get and Redistribute the Data

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

## set global and local dimensions
g.dim <- c(64, 64, 1024)
my.dim <- g.dim / c(1, 1, comm.size())

save.file <- paste("xyz.RData", comm.rank(), sep="")
load(save.file)    # gets vx vector

## reshape 3d array into a matrix
## first two dimensions become rows and third becomes columns

## local reshape dimensions
my.nrow <- prod(my.dim[1:2])
my.ncol <- my.dim[3]
ldim <- c(my.nrow, my.ncol)

## global reshape dimensions
g.nrow <- prod(g.dim[1:2])
g.ncol <- g.dim[3]
gdim <- c(g.nrow, g.ncol)

## now reshape local
X <- matrix(vx, nrow=my.nrow, ncol=my.ncol, byrow=FALSE)

## glue local pieces into a ddmatrix
X <- new("ddmatrix", Data=X, dim=gdim, ldim=ldim, bldim=ldim, ICTXT=1)

## transform to 2d block cyclic
X <- redistribute(X, bldim=c(8,8), ICTXT=0)

## Plot few columns in parallel
   . . .
finalize()
```

Plots in parallel

Make comm.size() plots in parallel

```
step <- 5
max.plots <- min(20, ncol(X) %/% step)
last.plot <- 1 - step
time <- comm.timer(
for(i in 1:max.plots)
    {
        now.plots <- last.plot + step*(1:comm.size())
        my.col <- gather.col(X[, now.plots])
        lab <- paste("col", lead0(now.plots[comm.rank()
            + 1]), sep="")
        png.slice(my.col, g.dim[1:2], lab)
        last.plot <- now.plots[length(now.plots)]
    }
)
```

Plots in parallel

gather.col First Attempt (1_plot.r)

```
gather.col <- function(x, num=min(ncol(x), comm.size()))
{
    ## gather complete columns of a global array to different ranks
    my.local <- as.vector(x[, comm.rank() + 1], proc.dest=comm.rank())
    my.local
}
```

Plots in parallel

gather.col Second Attempt (2_plot.r)

```
gather.col <- function(x, num=min(ncol(x), comm.size()))
{
  ## gather complete columns of a global array to
      different ranks
  my.local <- NULL
  for(i in 1:num)
    {
      ## serial collection of unique data to each rank
      local <- as.vector(x[, i])
      if(comm.rank() + 1 == i) my.local <- local
    }
  my.local
}
```

Plots in parallel

gather.col The Right Way (3_plot.r)

```
gather.col <- function(x, num=min(ncol(x), comm.size()))
{
  ## gather complete columns of a global array to
      different ranks
  x.num <- x[, 1:num]
  x.num <- as.colblock(x.num)

  ## ScaLAPACK fix (a future release will automate)
  if(ownany(x.num))
    ret <- as.vector(submatrix(x.num))
  else
    ret <- NULL
  ret
}
```

Plots in parallel

Now Plot the PCA Components (4_plot.r)

```
E <- sqrt(X^2 + Y^2 + Z^2)

E.pca <- prcomp(x=E, retx=TRUE, scale=FALSE)

## Use ranks 1 to n.pca to plot individual components in parallel
n.pca <- min(comm.size(), g.nrow)
my.col <- gather.col(E.pca$x, num=n.pca)

if(!is.null(my.col))
  {
    ## component plots on rank 1 to n.pca
    lab <- paste("pc", comm.rank(), sep="")
    title <- paste(lab, "sigma^2 =", variance[comm.rank() + 1])
    png.slice(my.col, g.dim[1:2], lab, title=title, work.dir=work.dir)
  }
```

SimpleRedistributions

- as.block(dx, square.bldim = TRUE)
- as.rowblock(dx)
- as.colblock(dx)
- as.rowcyclic(dx, bldim = .BLDIM)
- as.colcyclic(dx, bldim = .BLDIM)
- as.blockcyclic(dx, bldim = .BLDIM)

BLACS context (Processor Grid)

- init.grid(P,Q)
- .ICTXT = 0 gives P x Q
- .ICTXT = 1 gives PQ x 1
- .ICTXT = 2 gives 1 x PQ

Exercise: scripts/pbdDMAT/dmat_app

- Experiment with scripts 0_pca.r, 1_plot.r, 2_plot.r, 3_plot.r, 4_plot.r, 5ictxt.r, 6_ictxt.r, and 7_ictxt.r
- Experiment with other redistributions

Contents

11 Wrapup

The pbdR Project

- Our website: http://r-pbd.org/
- Email us at: RBigData@gmail.com
- Our google group: http://group.r-pbd.org/

Where to begin?

- The **pbdDEMO** package http://cran.r-project.org/web/packages/pbdDEMO/
- The **pbdDEMO** Vignette: http://goo.gl/HZkRt

Thanks for coming!

Questions?

pbdR
Programming with Big Data in R

http://r-pbd.org/