Introduction to parallel computing with R - pbdMPI

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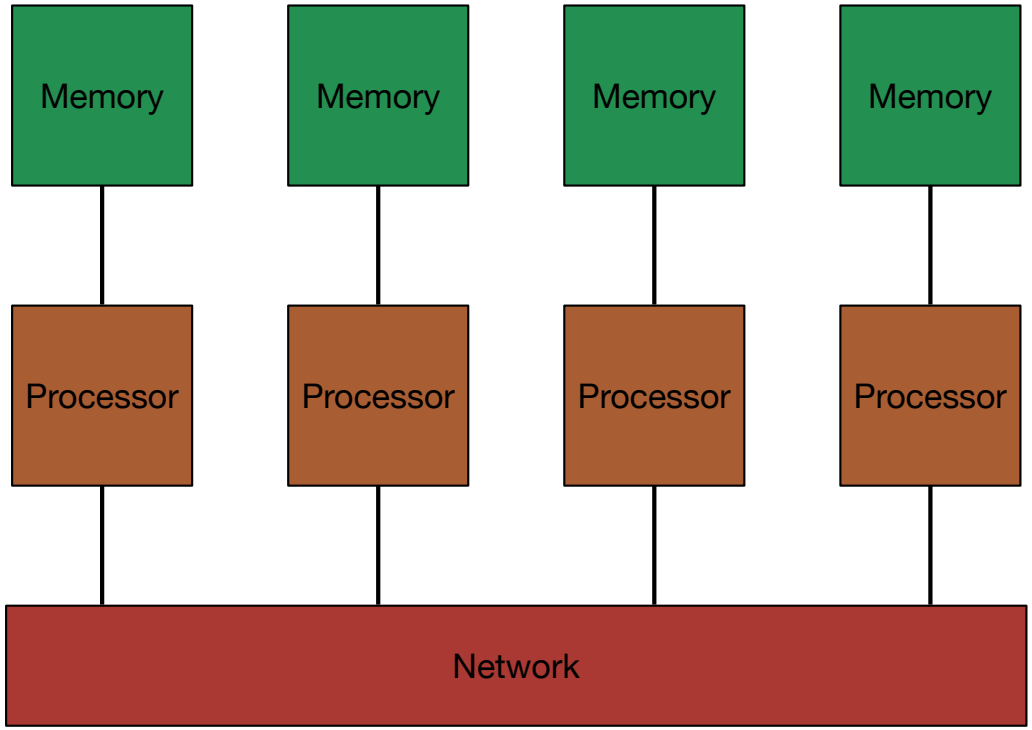
https://github.com/ResearchComputing/RMACC
https://github.com/ResearchComputing/RMACC/blob/master/2017/Parallel_R/03-R-distributed.pdf

Outline

- Distributed parallel computing
- Quick overview over MPI (Message Passing Interface)
- Package pbdMPI
- Examples
  - Hello World
  - PI

Distributed Memory Computer

- Processors have different content in memory
- Data exchange by message passing



Execution

- You can run a MPI program with the following commands

```
$ mpirun –n 24 Rscript yourRprogram.R
```

Run hello_print.R

- Example – Run the hello_print.R

```
$ sinteractive --partition=shas --qos=debug \
--time=30:00 --ntasks=10 --nodes=2 \
--reservation=parallel-r
$ module purge
$ module load R
$ module load openmpi
$ cd $HOME/RMACC/Parallel_R/examples/pbdMPI
$ mpirun -n 10 Rscript hello_print.R
```

- Vary –n (needs to be lower than --ntasks)
- Is the output always in the same order?

Programming in MPI

```
library(pbdMPI, quiet=TRUE)

init()
.
.
.
finalize()
```

```
#include “mpi.h”

int ierr;
ierr = MPI_Init(&argc, &argv);
.
.
.
ierr = MPI_Finalize();
```

MPI Communicator

- A collection of processors of an MPI program
- Used as a parameter for most MPI calls.
- Processors with in a communicator have a number
  - Rank: 0 to n-1
- `comm`
  - Contains all processors of your program run
- You can create new communicators that are subsets
  - All even processors
  - The first processor
  - All but the first processor

Programming in MPI

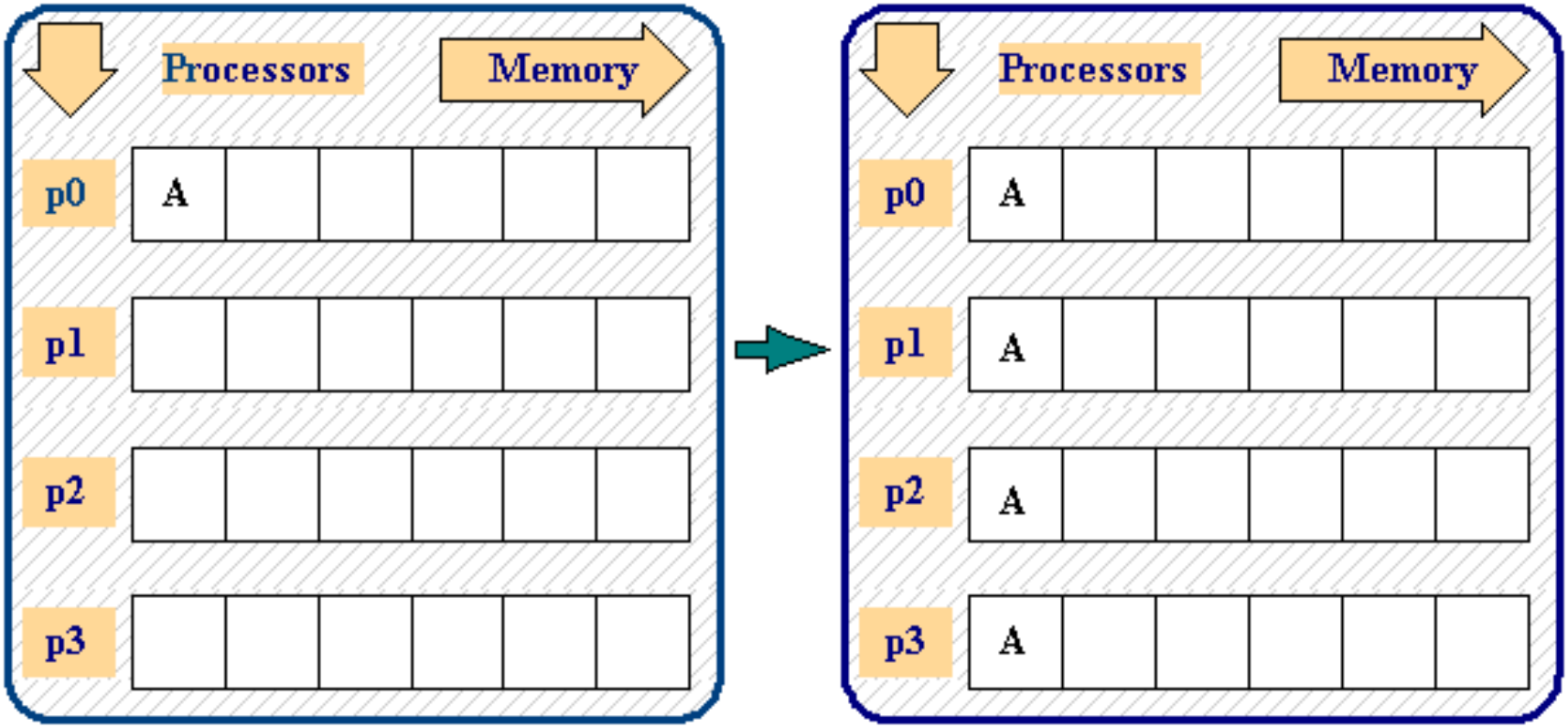
```
library(pbdMPI, quiet = TRUE)

init()

nprocs <- comm.size()
id <- comm.rank().
.
.
finalize()
```

Determine process id or *rank* (here = id)
And number of processes (here = nprocs)

Package pdbMPI

- Implements interface to MPI
  - `> comm.print(variable, all.rank=TRUE)`
  - `> comm.size()`
  - `> comm.rank()`
  - `> comm.set.seed(diff=TRUE)`
  - `> pbdApply(X, margin, func, …)`
  - `> pbdLapply(X, func, ...)`
  - `> pbdSapply(X, fun, …)`
  - `> bcast`
  - `> allgather`
  - `> reduce`

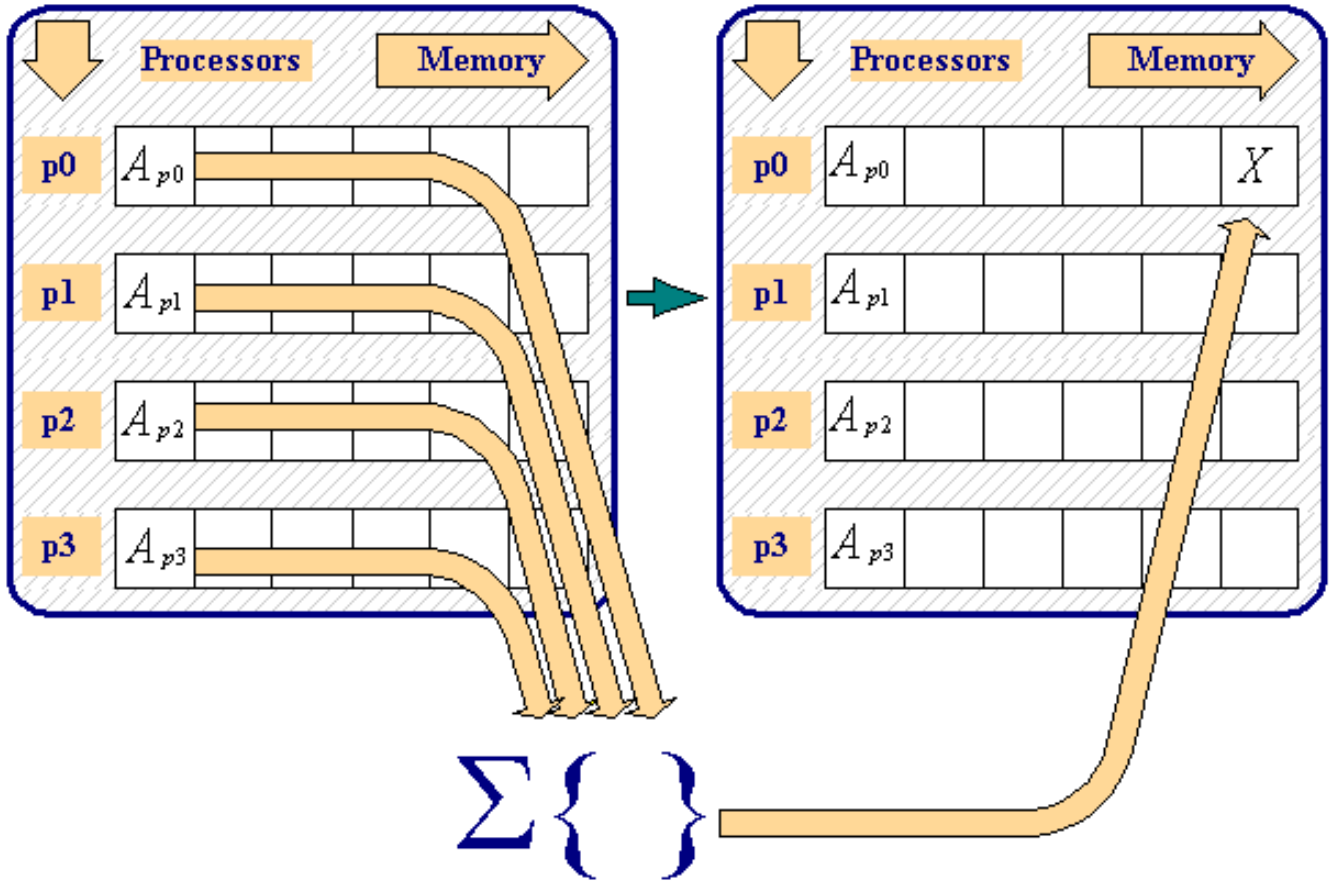
Broadcast




```
send_count = 1;
  root = 0;
  MPI_Bcast ( &a, send_count, MPI_INT, root, comm )
```

Figure from MPI-tutor: http://www.citutor.org/index.php

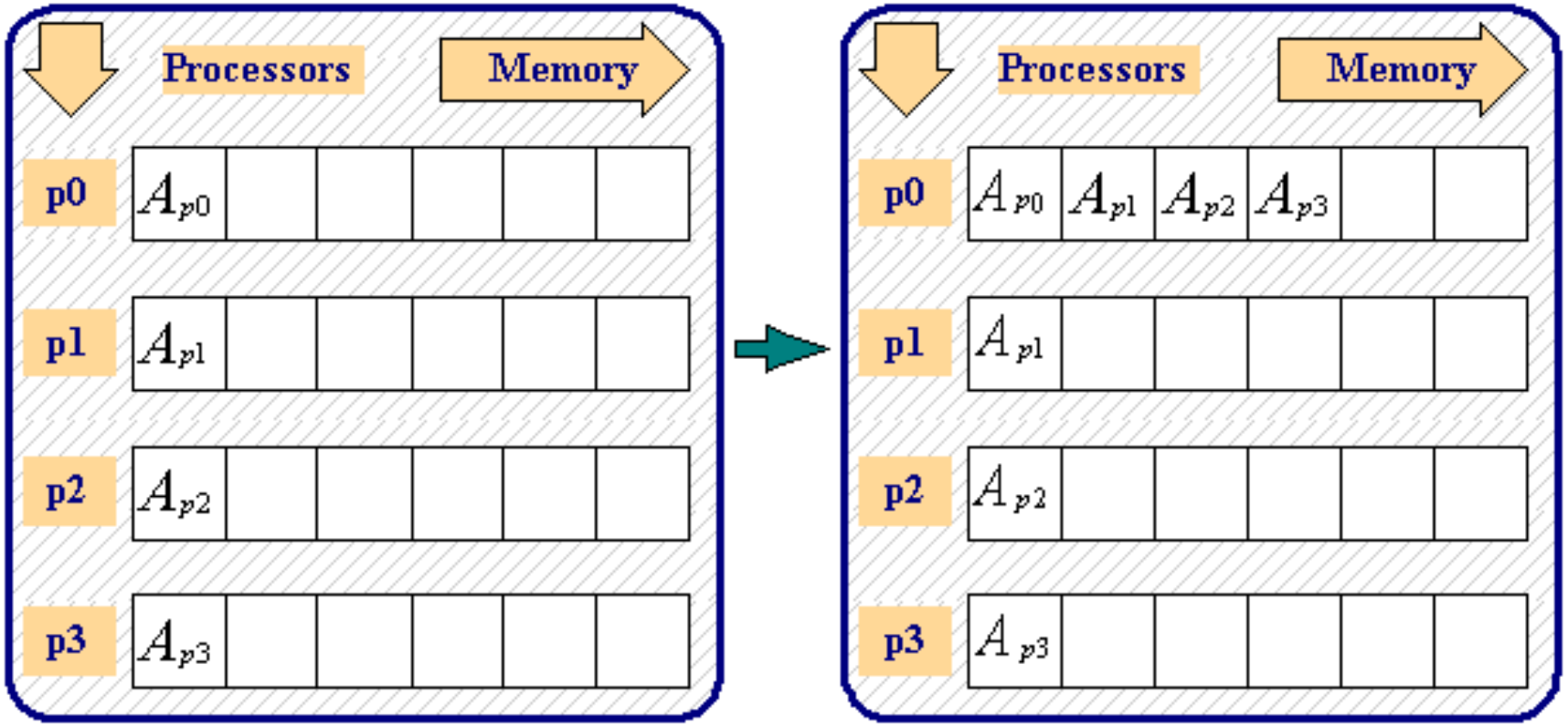
Reduction




```
count = 1;
rank = 0;
MPI_Reduce ( &a, &x, count, MPI_REAL, MPI_SUM, rank,  MPI_COMM_WORLD );
```

Figure from MPI-tutor: http://www.citutor.org/index.php

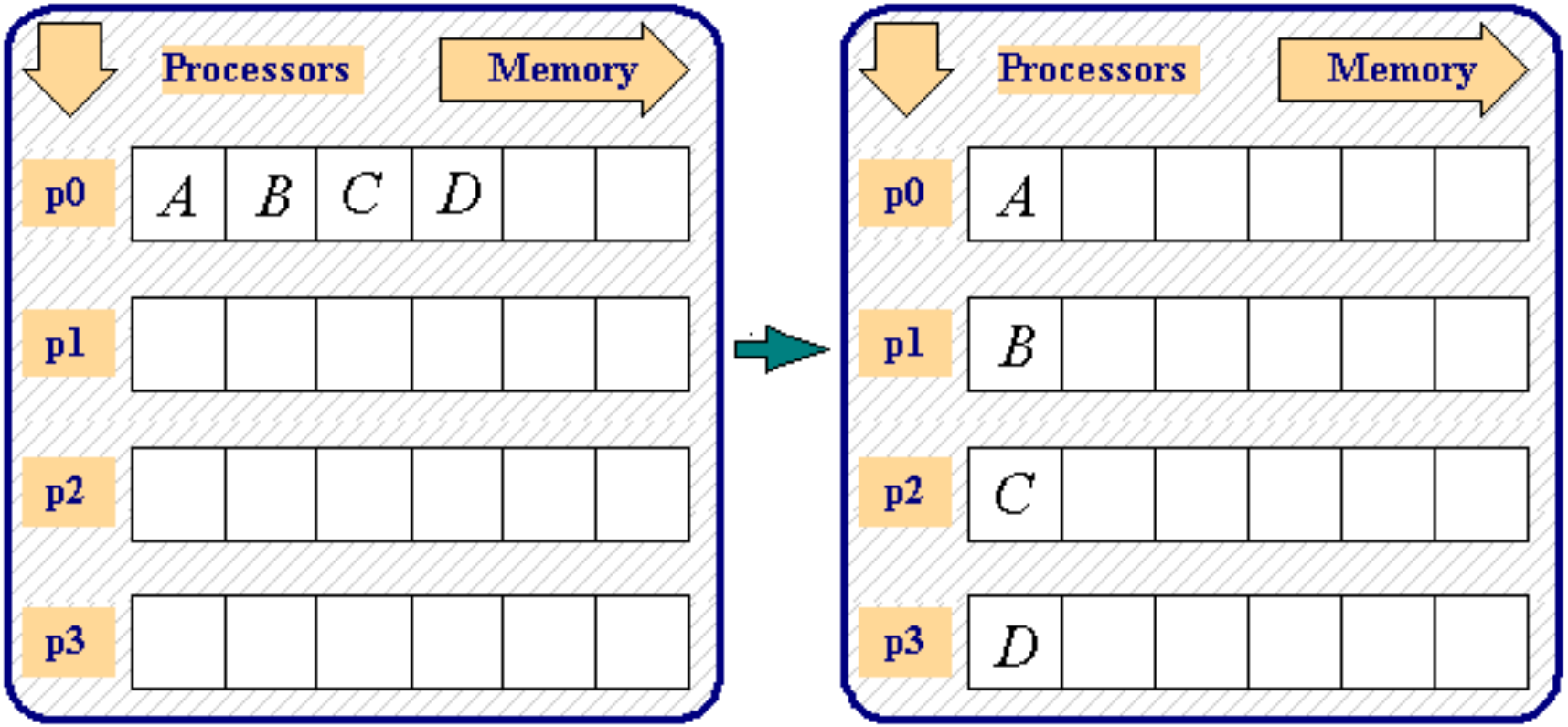
Gather




```
send_count = 1;
recv_count = 1;
recv_rank = 0;
MPI_Gather ( &a, send_count, MPI_REAL, &a, recv_count, MPI_REAL, recv_rank,
MPI_COMM_WORLD );
```

Figure from MPI-tutor: http://www.citutor.org/index.php

Scatter




```
recv_count = 1;
send_rank = 0;
MPI_Scatter ( &a, send_count, MPI_REAL,
              &a, recv_count, MPI_REAL,
              send_rank, MPI_COMM_WORLD );
```

Figure from MPI-tutor: http://www.citutor.org/index.php

Printing

- `> comm.print("String", all.rank=TRUE|FALSE)`
  - All processors have to participate
  - `all.rank=TRUE` – prints on all ranks
- Globally print or cat a variable from specified processors
- By default message is shown on screen
- Warning: uses a barrier, so needs to be called by all processors
  - DEADLOCK danger
  - Barrier is a synchronization between all processes. All processes have to join the call and processes wait until all have called it

Deadlock

- Deadlock: process waiting for a condition that will never become true
- Easy to write send/receive code that deadlocks
  - Two processes: both receive before send
  - Send tag doesn't match receive tag
  - Process sends message to wrong destination process

Exercise – hello_deadLock.R

- Run

```
$ mpirun -n 4 Rscript hello_deadLock.R
```

- What's happening?

- Try to fix the problem

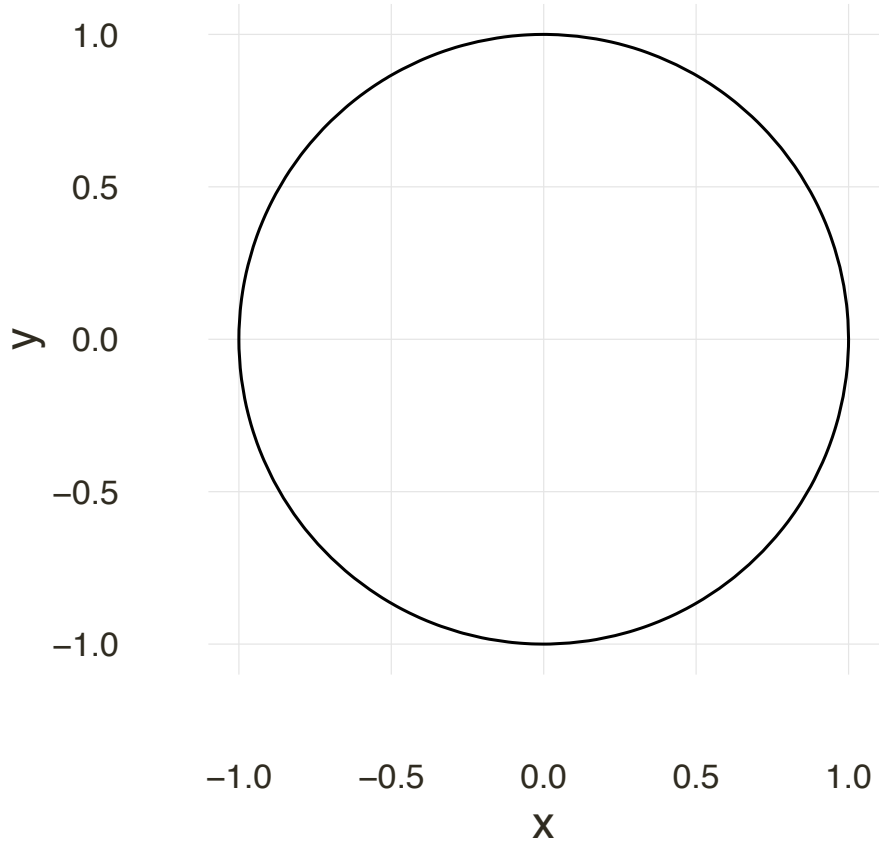
pbdApply, pbdSapply

```
$ pbdSapply(n, approx.pi, pbd.mode="spmd")
```

- `pbd.mode`
  - Single program multiple data – spmd
    - Need to distribute the data
      - Scatter or execute code on all processes
    - Need to collect the data
      - Gather or reduce
  - Master Worker – "mw"
    - Will distribute the first argument to the workers
    - Will get the result back
    - See later example

Calculate PI with Monte Carlo

- Goal: estimate the area of a circle with radius = 1 and area = π using Monte Carlo integration.



Exercise – pi_pbdSapply

- Is the program using the weak scaling or strong scaling approach?
- Run the program on your own node using
  - 4, 16 and 24 cores
- Modify the program so that it uses the other approach.

- result variable has no value after the reduce
  - How can we fix this?

Exercise – pi_mw_pbdSapply

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- Modify the program so that it uses the other approach.

- result variable has no value after the reduce
  - How can we fix this?

Questions?

- Email rc-help@colorado.edu
- Twitter: CUBoulderRC

- Slides:
  - https://github.com/ResearchComputing/RMACC/blob/master/2017/Parallel_R/03-R-setup.pdf

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