pbdR: Input, PCA, and Movies

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The pbdR Core Team

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pbdR
Programming with Big Data in R

Support

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Contents

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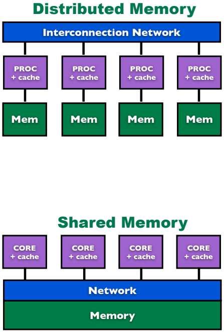
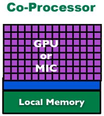
Three Basic Flavors of Hardware

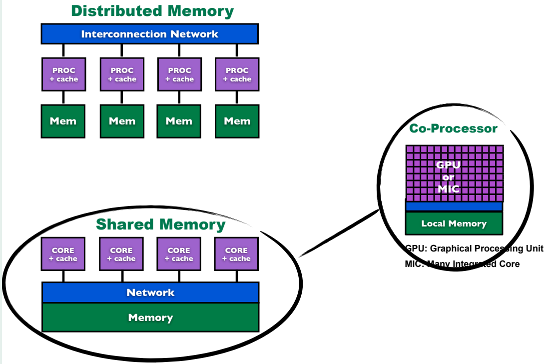




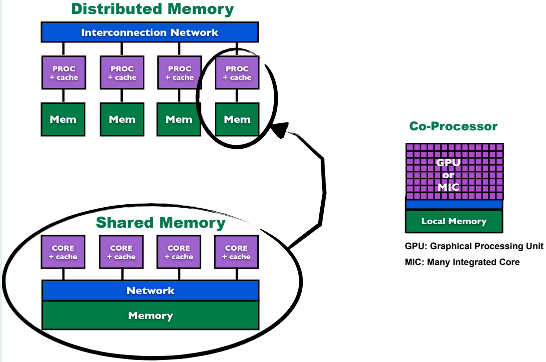
GPU: Graphical Processing Unit

MIC: Many Integrated Core

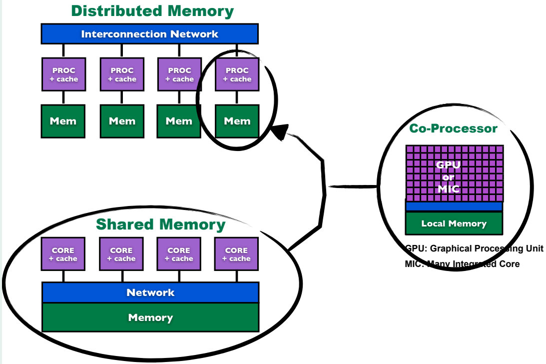
Your Laptop or Desktop



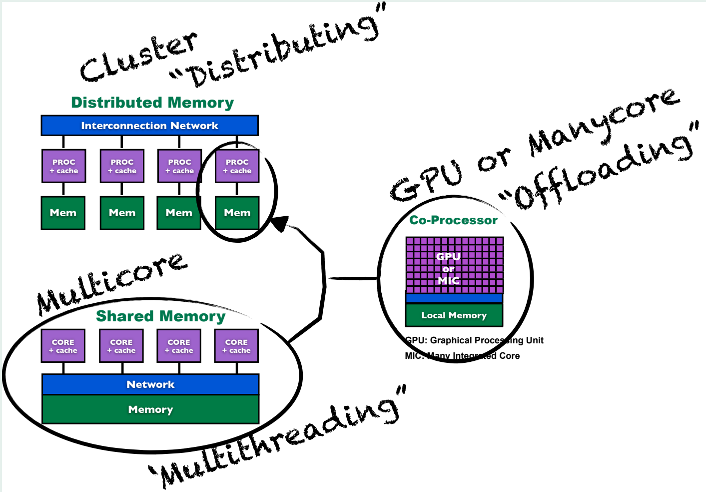
A Server or Cluster



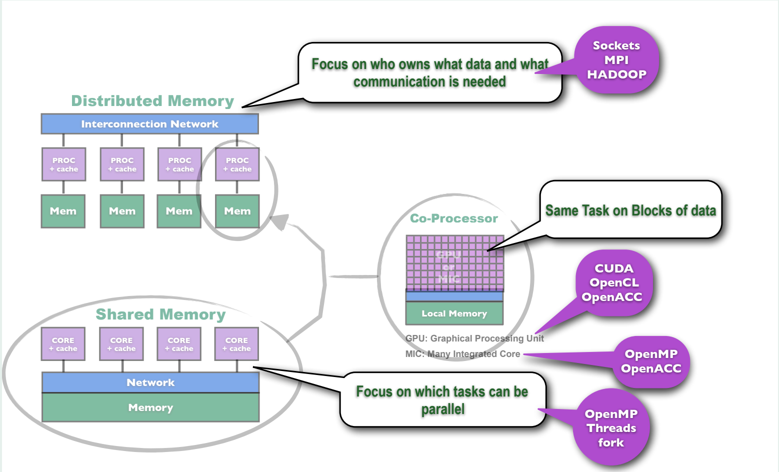
Server to Supercomputer



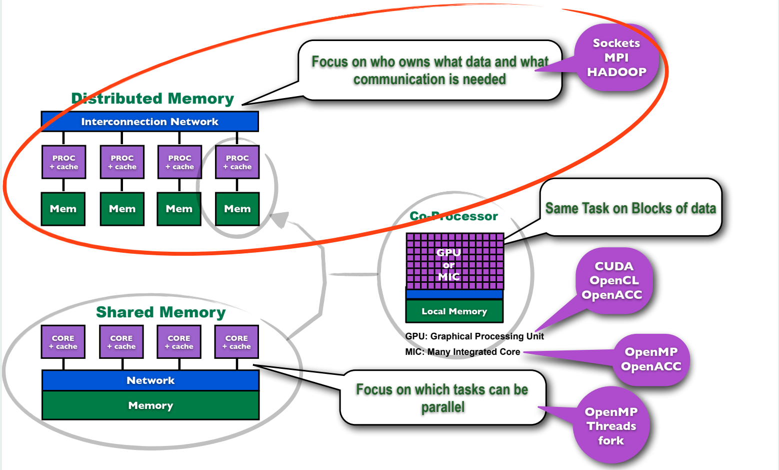
Knowing the Right Words



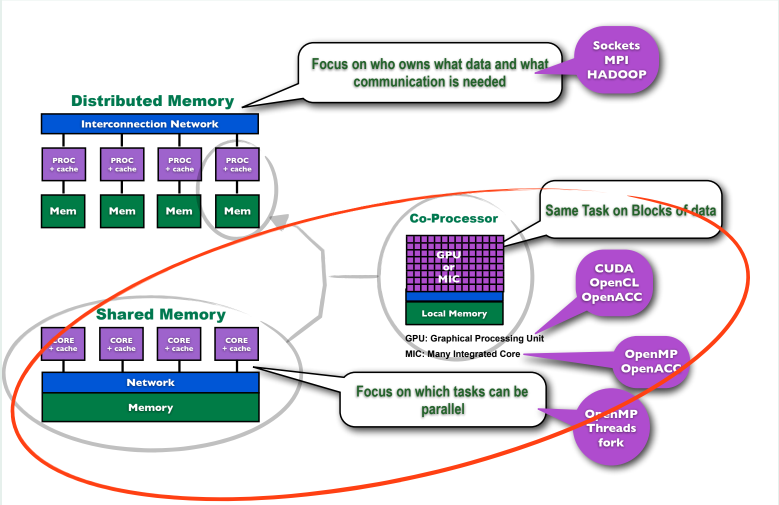
"Native" Programming Models and Tools



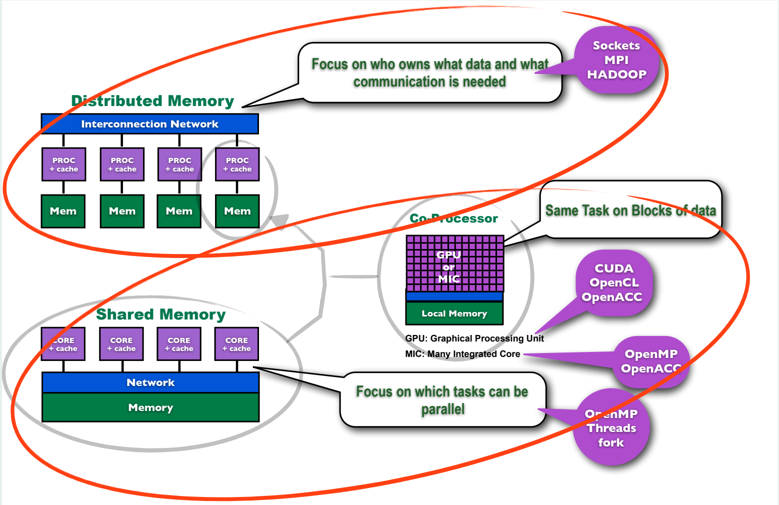
30+ Years of Parallel Computing Research



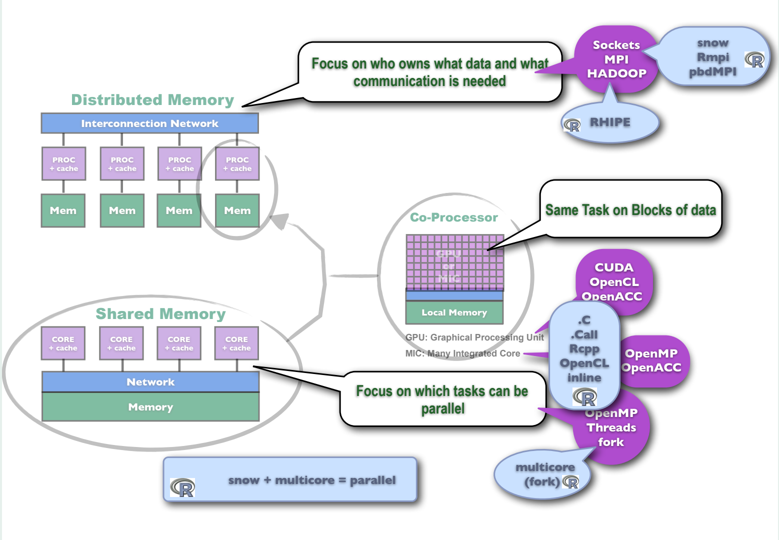
Last 10 years of Advances



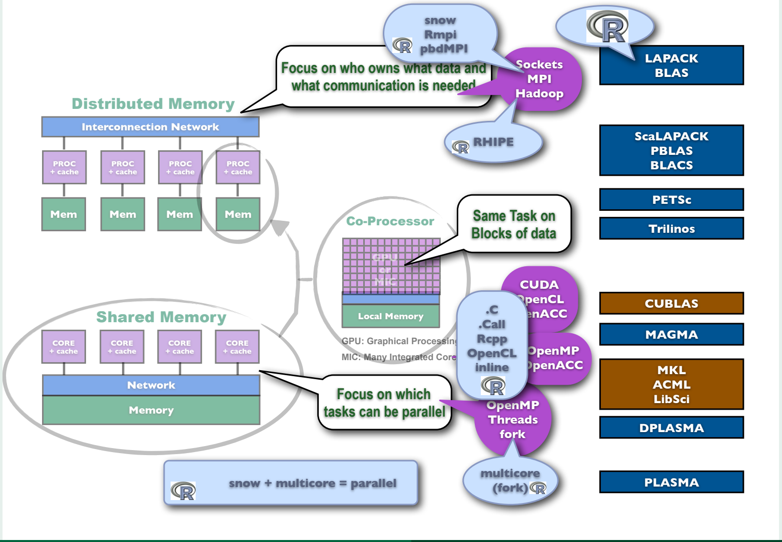
Putting It All Together Challenge



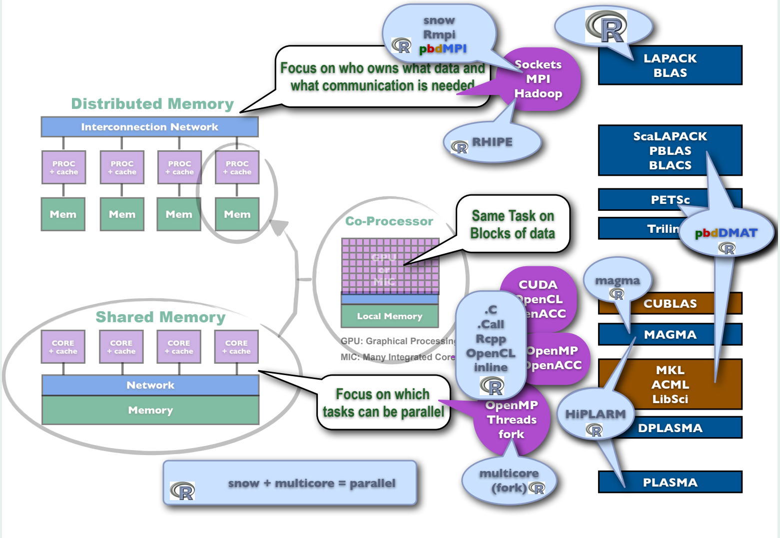
R Interfaces to Native Tools



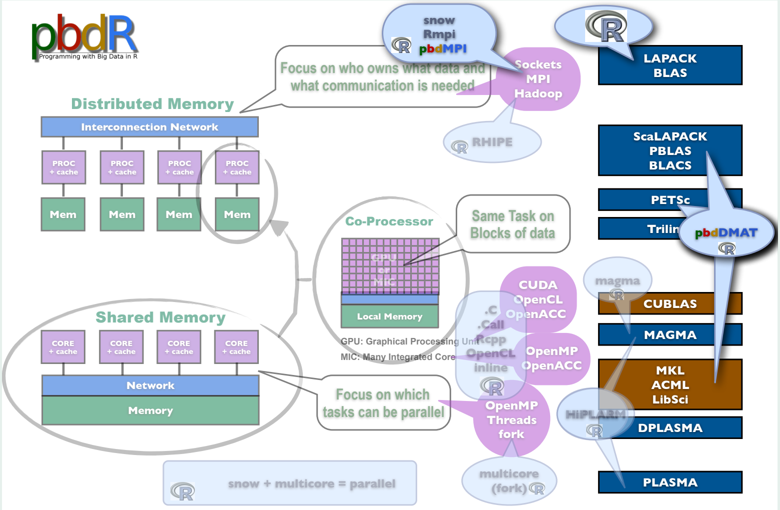
HPC Libraries



R Interfaces to Scalable HPC Libraries



pbdR Interfaces to Scalable HPC Libraries



Contents

I/O has a separate manual: http://r-project.org/

- scan()
- read.table()
- read.csv()
- ...
- readBin()
- ncvar_get()
- readSocket()

No parallel file system: Read Serial then Distribute

read.csv()

```
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?
- ...
- Currently very "hands on"
- 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()
```

NetCDF4 Data

Parallel Read

```
### 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

Binary Data

Read subcube

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

data.dim <- c(2048, 2048, 2048) # full data dimension
g.start <- c(1, 1, 513)         # global subcube corner
g.dim <- c(64, 64, 1024)        # global subcube extent

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

size <- 4 # file is single precision floats

vx <- block3d.read(``filename'', data.dim, my.start,
    my.dim, size)

## 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)

## 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)
```

Binary Data

3d Block Binary Reader

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

  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
  }

  close(con.x)
  x
}
```

Contents

The Math

$m \times n$ matrix X: Measurements on n spatial locations at m times

Center the matrix: X_c is the column centered X

Singular value decomposition: $X_c = VDU^T$

n time series: columns of $VD = X_c U$

m images: columns of $UD = X_c^T V$

Note that VD and UD have same units as X

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)

```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()
```

Contents

How can we plot in parallel?

- Several plots, one or more on each processor (can do now)
- One plot by several processors (need to rewrite graphics)

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 (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)
  }
```

Exercise: scripts/pbdDMAT/dmat_app

- Experiment with scripts 0_pca.r, 1_plot.r, 2_plot.r, 3_plot.r, 4_plot.r

Contents

Simple Redistributions

- 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 5ictxt.r, 6_ictxt.r, and 7_ictxt.r
- Experiment with other redistributions

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/