Programming with Big Data in R

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Oak Ridge National Laboratory

2016 OLCF User Meeting: Day 0 Tutorial

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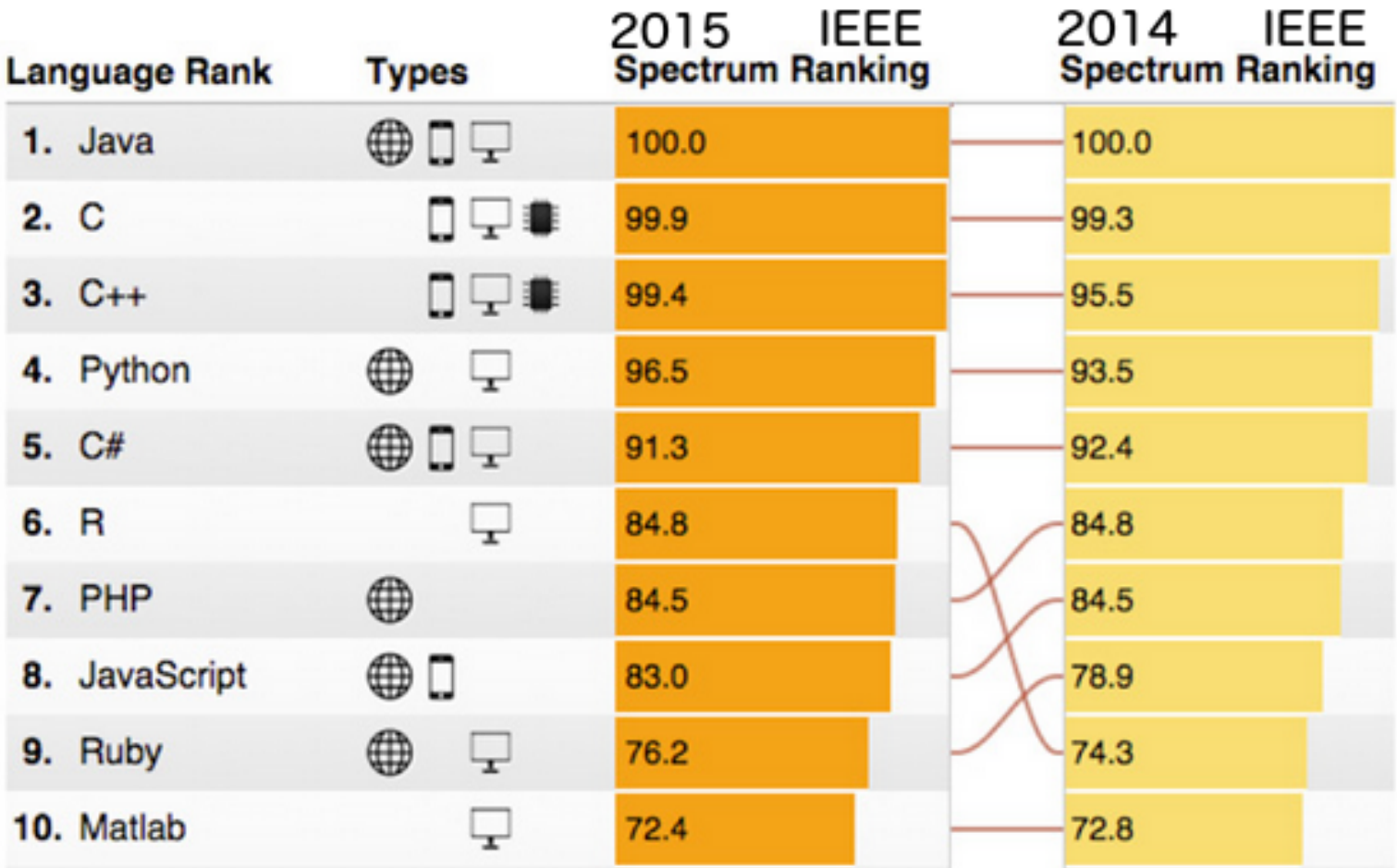
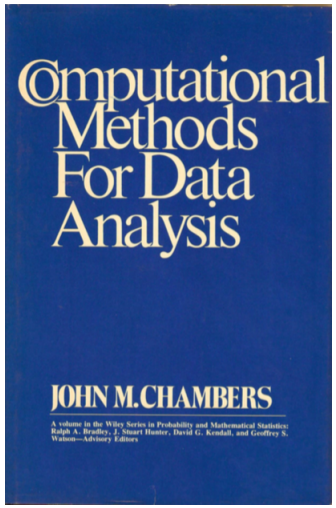
Why R? Popularity?

IEEE Spectrum's Ranking of Programming Languages

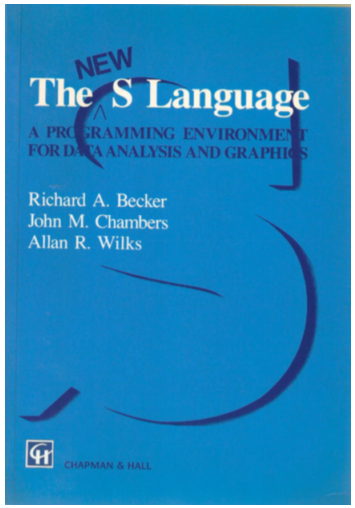


See: http://spectrum.ieee.org/static/interactive-the-top-programming-languages#index

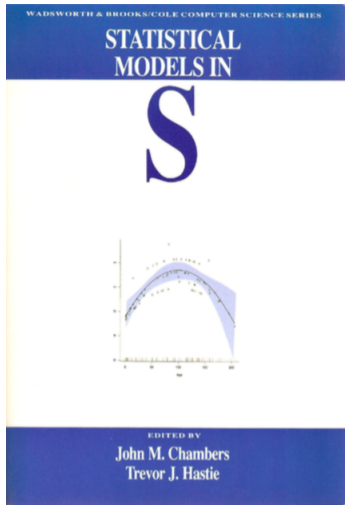
Why R? Programming with Data



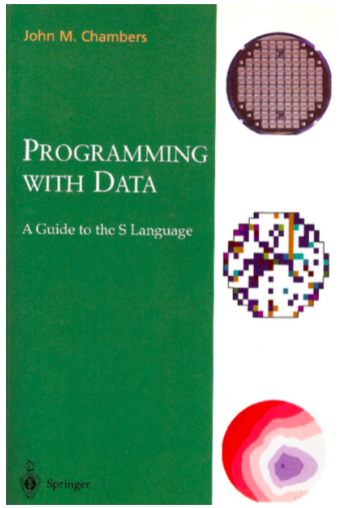
Chambers. *Computational Methods for Data Analysis*. Wiley, 1977.



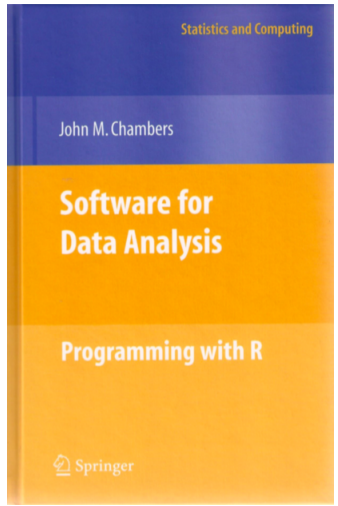
Becker, Chambers, and Wilks. *The New S Language*. Chapman & Hall, 1988.



Chambers and Hastie. *Statistical Models in S*. Chapman & Hall, 1992.



Chambers. *Programming with Data*. Springer, 1998.



Chambers. *Software for Data Analysis: Programming with R*. Springer, 2008.

Thanks to Dirk Eddelbuettel for this slide idea and to John Chambers for providing the high-resolution scans of the covers of his books.

Why R? Resources for Learning R

- RStudio IDE
  http://www.rstudio.com/products/rstudio-desktop/
- *Task Views*: http://cran.at.r-project.org/web/views
- Book: *The Art of R Programming* by Norm Matloff:
  http://nostarch.com/artofr.htm
- *Advanced R*: http://adv-r.had.co.nz/ and *ggplot2*
  http://docs.ggplot2.org/current/ by Hadley Wickham
- R programming for those coming from other languages: http://www.johndcook.com/R_language_for_programmers.html
- *aRrgh: a newcomer's (angry) guide to R*, by Tim Smith and Kevin Ushey: http://tim-smith.us/arrgh/
- Mailing list archives: http://tolstoy.newcastle.edu.au/R/
- The [R] stackoverflow tag.

Why R? Programming with Big Data

pbdR Core Team
Wei-Chen Chen, FDA
George Ostrouchov, ORNL & UTK
Drew Schmidt, UTK

Developers
Christian Heckendorf, Pragneshkumar Patel, Gaurav Sehrawat

Contributors
Whit Armstrong, Ewan Higgs, Michael Lawrence, David Pierce, Brian Ripley, ZhaoKang Wang, Hao Yu

- Engage parallel libraries at scale
- R language unchanged
- New distributed concepts
- New profiling capabilities
- New interactive SPMD
- In situ distributed capability
- In situ staging capability via ADIOS
- Plans for DPLASMA GPU capability

Modules on Titan, Rhea, and Eos (Current R Version is 3.3.0)

Notes - Remember to submit R to compute nodes and not run it on login nodes
Notes - R gpu code can run on Titan nodes or Rhea gpu nodes

```
module load r/3.3.0
R
rstudio ( Currently only on Rhea - use either a remote visualization tool or forward
      X [ssh -X and qsub -X] )
```

Example qsub batch script for Titan

```
#!/bin/csh
#PBS -A STF006
#PBS -N R
#PBS -q batch
#PBS -l nodes=1
#PBS -l walltime=0:15:00

cd /lustre/atlas2/stf006/world-shared/mikem

module load r/3.3.0

setenv OPENBLAS_NUM_THREADS 1
setenv OMP_NUM_THREADS 1

echo "host = `hostname`"

aprun -n 1 Rscript --vanilla eigen.r
aprun -n 1 Rscript --vanilla ex_hdf5.r
aprun -n 1 Rscript --vanilla ex_max.r
```

Strategies for Making R, a Scripting Language, Faster

Serial solutions before parallel solutions

- User R code often inefficient (high-level code = deep complexity)
  - Profile and improve code first
  - Vectorize loops if possible
  - Compute once if not changing
  - Know when copies are made
- Move kernels into compiled language, such as C/C++ (+OpenMP)
- **multicore** components of **parallel** package (Unix fork)
- Distributed via pbdR (only solution for big memory)

Integrating C/C++ Code Into R

`.Call`

- Standard R interface to C code
- Lightweight but clunky

Rcpp: Incorporating C++ code into R

Authors: Dirk Eddelbuettel and Romain Francois

- Simplifies integrating C++ code with R
- Maps R objects (vectors, matrices, functions, environments, . . .) to dedicated C++ classes
- Broad support for C++ Standard Template Library idioms.
- C++ code can be compiled, linked and loaded on the fly, or added via packages.
- Error and exception code handling

Rcpp Example: A simple row max calculation

cat ex_max.cpp

```
1  #include <Rcpp.h>
2  using namespace Rcpp;
3
4  //[[Rcpp::export]]
5
6  NumericVector row_max( NumericMatrix m )
7  {
8     int nrows = m.nrow( );
9     NumericVector maxPerRow( nrows );
10
11    for ( int i = 0; i < nrows; i++ )
12    {
13       maxPerRow[ i ] = Rcpp::max( m( i, _ ) );
14    }
15
16    return ( maxPerRow );
17 }
```

One can get configuration values by

```
1  setenv PKG_CXXFLAGS  `Rscript -e "Rcpp:::CxxFlags( )"`
2  setenv PKG_LIBS `Rscript -e "Rcpp:::LdFlags( )"`
```

Rcpp Example (con'd): A simple row max calculation

cat ex_max.r

```
1  library( Rcpp )
2  Sys.setenv( "PKG_CXXFLAGS" =
3   "-I /sw/redhat6/r/3.3.0/rhel6_gnu4.8.2/lib64/R/library/Rcpp/include" )
4  Sys.setenv( "PKG_LIBS"="-lm" )
5
6  sourceCpp( "ex_max.cpp" )
7
8  set.seed( 27 )
9  X <- matrix( rnorm( 4 * 4 ), 4, 4 )
10 X
11
12 print( "Rcpp" )
13 row_max( X )
```

Rscript ex_max.r

```
1  Rscript ex_max.r
2              [,1]          [,2]         [,3]        [,4]
3  [1,]  1.9071626 -1.093468881  2.13463789  1.5702953
4  [2,]  1.1448769  0.295241218  0.23784461  0.1580101
5  [3,] -0.7645307  0.006885942 -1.28512736 -0.7457995
6  [4,] -1.4574325  1.157410886  0.03482725 -1.0688030
7  [1] "Rcpp"
8  [1] 2.134637891 1.144876890 0.006885942 1.157410886
```

- The RcppArmadillo package is a set of bindings to the Armadillo C++ library.
- Armadillo is a templated C++ linear algebra library that uses supplied BLAS and LAPACK.
- Includes some machine learning libraries
- BLAS and LAPACK are also directly engaged from R.
- Probably not faster than R direct but not having to come back out to R if C++ code needs to use linear algebra can produce gains.

RcppArmadillo Example: Eigenvalue calculation

cat eigen.cpp

```
1 #include <RcppArmadillo.h>
2 //[[Rcpp::depends(RcppArmadillo)]]
3 //[[Rcpp::export]]
4
5 arma::vec getEigenValues( arma::mat M )
6 {
7     return ( arma::eig_sym( M ) );
8 }
```

RcppArmadillo Example (con'd): Eigenvalue calculation

cat eigen.r

```
1  library( Rcpp )
2  library( RcppArmadillo )
3  Sys.setenv( "PKG_CXXFLAGS" = "-I
       /sw/redhat6/r/3.3.0/rhel6_gnu4.8.2/lib64/R/library/RcppArmadillo/include" )
4  Sys.setenv( "PKG_LIBS"="-lm"
5  )
6  sourceCpp( "eigen.cpp" )
7
8  set.seed( 27 )
9  X <- matrix( rnorm( 4 * 4 ), 4, 4 )
10 Z <- X %*% t( X )
11 print( "RcppArmadillo" )
12 getEigenValues( Z )
13
14 print( "R" )
15 eigen( Z )$values
```

Rscript eigen.r

```
1  [1] "RcppArmadillo"
2               [,1]
3  [1,]  0.03779289
4  [2,]  0.85043786
5  [3,]  2.03877658
6  [4,] 17.80747601
7  [1] "R"
8  [1] 17.80747601  2.03877658  0.85043786  0.03779289
```

I/O

I/O Packages

- function `fread` in package **data.table**: fast and easy `csv`
- **rhdf5**: fast and easy HDF5 I/O
- **pbdNCDF4**: fast NetCDF4 collective read and write
- **pbdADIOS** (on GitHub, under developent): fast `bp` I/O with ADIOS staging capability
- **pbdIO** (on GitHub, under development): Easy parallel I/O, includes parallel `csv` with load balance

Parallel chunking: Read the most natural way from disk

- C: by blocks of rows
- FORTRAN: by blocks of columns
- CSV best with groups of files
- Parallel best with binary, fixed format

rhdf5 Example: Write and then read a matrix

cat wr_hdf5.r

```
1  library( rhdf5 )
2  print( "Writing hdf5" )
3  h5createFile( "test.h5" )
4  h5createGroup( "test.h5", "MainGroup" )
5  X <- matrix( rnorm( 3 * 3 ), ncol = 3, nrow = 3 )
6  X
7  h5write( X, file = "test.h5", "MainGroup/Matrix", write.attributes = FALSE )
8  h5ls( "test.h5" )
9  print( "Reading hdf5" )
10 Y <- h5read( "test.h5", "/MainGroup/Matrix" )
11 Y
```

Rscript wr_hdf5.r

```
1  Loading required package: methods
2  [1] "Writing hdf5"
3  [1] TRUE
4  [1] TRUE
5             [,1]       [,2]       [,3]
6  [1,]  0.9124038  1.0390048 -1.1731370
7  [2,] -0.8973774  0.3447025 -0.1201449
8  [3,]  1.6489298 -0.1993730  1.1330055
9        group       name        otype dclass   dim
10 0         / MainGroup   H5I_GROUP
11 1 /MainGroup     Matrix H5I_DATASET  FLOAT 3 x 3
12 [1] "Reading hdf5"
13            [,1]       [,2]       [,3]
14 [1,]  0.9124038  1.0390048 -1.1731370
15 [2,] -0.8973774  0.3447025 -0.1201449
16 [3,]  1.6489298 -0.1993730  1.1330055
```

rhdf5 Example (con'd): Check file contents outside of R

h5dump test.h5

```
HDF5 "test.h5" {
GROUP "/" {
   GROUP "MainGroup" {
      DATASET "Matrix" {
         DATATYPE  H5T_IEEE_F64LE
         DATASPACE  SIMPLE { ( 3, 3 ) / ( 3, 3 ) }
         DATA {
         (0,0): 0.912404, -0.897377, 1.64893,
         (1,0): 1.039, 0.344703, -0.199373,
         (2,0): -1.17314, -0.120145, 1.13301
         }
      }
   }
}
}
```

Note: **rhdf5** enables reading chunks and slabs of HDF5 file arrays in R for fast parallel reads from the lustre file system.

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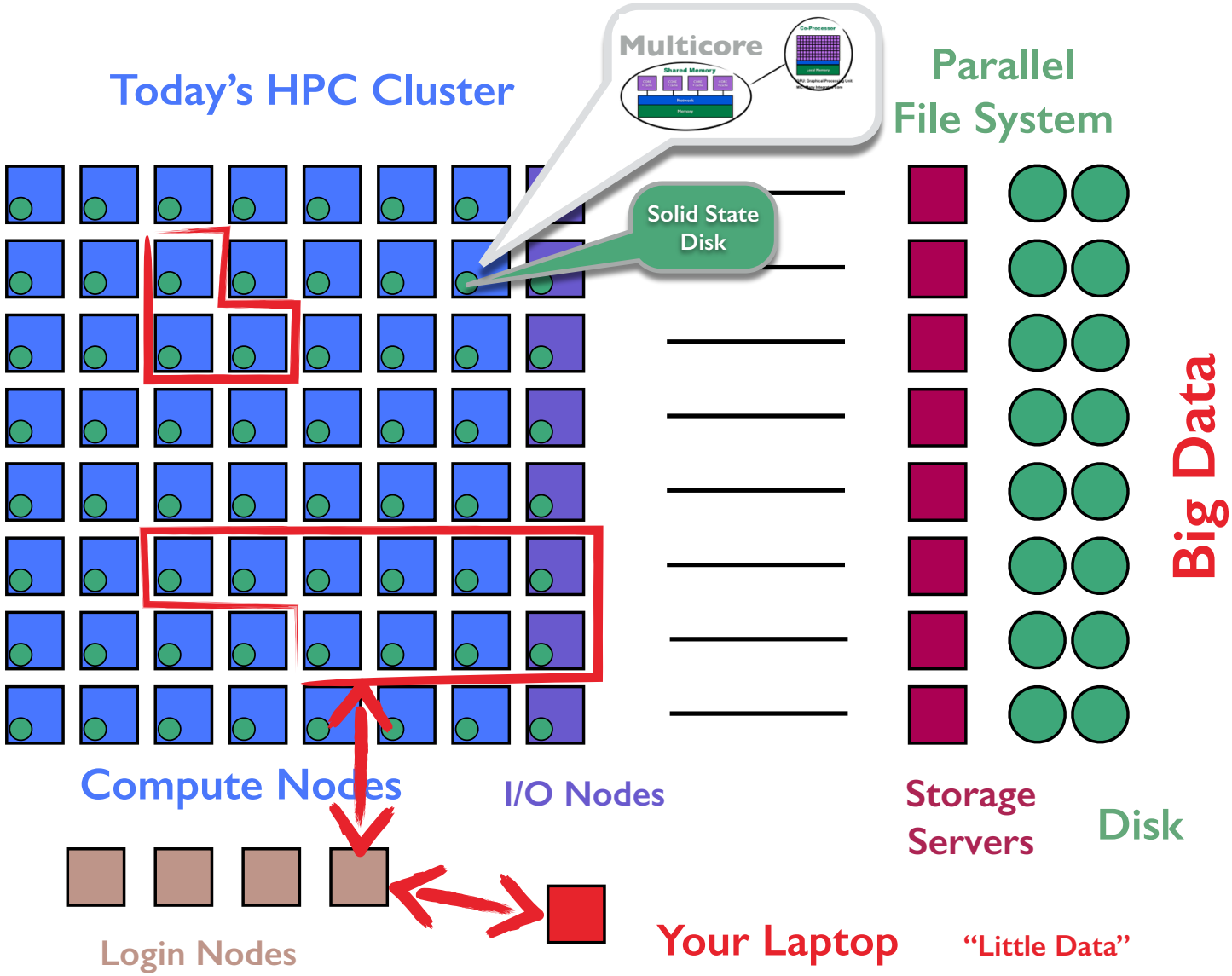
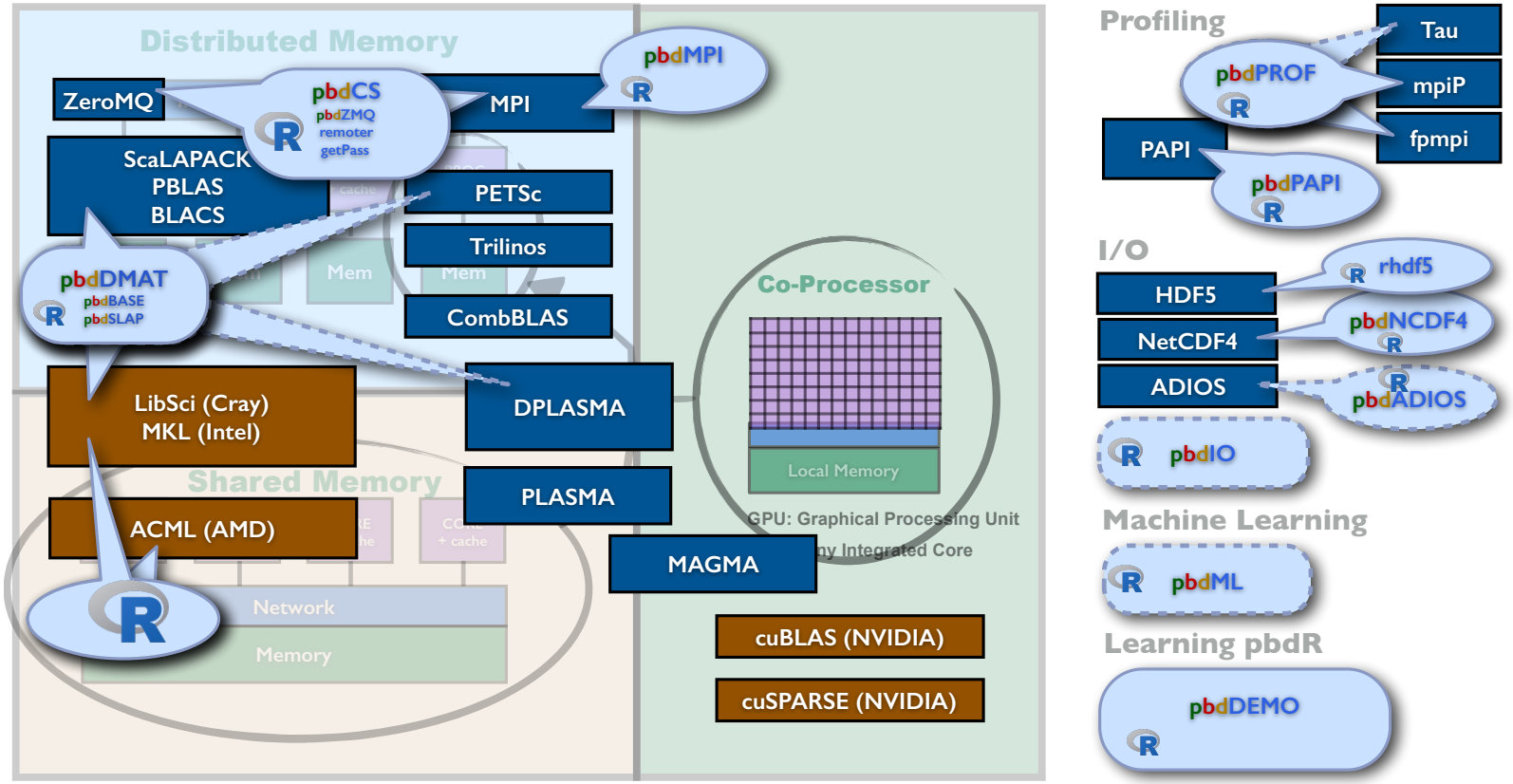
HPC Cluster with NVRAM and Parallel File System



pbdR Interfaces to Libraries: Sustainable Path



Why use HPC libraries?

- Many science communities are invested in their API.
- Data analysis uses much of the same basic math as simulation science
- The libraries represent 30+ years of parallel algorithm research
- *They're tested. They're fast. They're scalable.*

pbdMPI: a High Level Interface to MPI

- API is simplified: defaults in control objects.
- S4 methods: extensible to complex R objects.
- Additional error checking
- Array and matrix methods without serialization: faster than **Rmpi**.

pbdMPI (S4)	**Rmpi**
allreduce	mpi.allreduce
allgather	mpi.allgather, mpi.allgatherv, mpi.allgather.Robj
bcast	mpi.bcast, mpi.bcast.Robj
gather	mpi.gather, mpi.gatherv, mpi.gather.Robj
recv	mpi.recv, mpi.recv.Robj
reduce	mpi.reduce
scatter	mpi.scatter, mpi.scatterv, mpi.scatter.Robj
send	mpi.send, mpi.send.Robj

SPMD: Copies of One Code Run Asynchronously

A simple SPMD `allreduce`

allreduce.r

```
1  library(pbdMPI, quiet = TRUE)
2
3  ## Your local computation
4  n <- comm.rank() + 1
5
6  ## Now "Reduce" and give the result to all
7  all_sum <- allreduce(n) # Sum is default
8
9  text <- paste("Hello: n is", n, "sum is", all_sum )
10 comm.print(text, all.rank=TRUE)
11
12 finalize()
```

Execute this batch script via:

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

Output:

```
1 COMM.RANK = 0
2 [1] "Hello: n is 1 sum is 3"
3 COMM.RANK = 1
4 [1] "Hello: n is 2 sum is 3"
```

Machine Learning Example: Random Forest

Example: Letter Recognition data from package **mlbench** (20,000 × 17)

```
 1  [,1]    lettr    capital letter
 2  [,2]    x.box    horizontal position of box
 3  [,3]    y.box    vertical position of box
 4  [,4]    width    width of box
 5  [,5]    high     height of box
 6  [,6]    onpix    total number of on pixels
 7  [,7]    x.bar    mean x of on pixels in box
 8  [,8]    y.bar    mean y of on pixels in box
 9  [,9]    x2bar    mean x variance
10  [,10]   y2bar    mean y variance
11  [,11]   xybar    mean x y correlation
12  [,12]   x2ybr    mean of x^2 y
13  [,13]   xy2br    mean of x y^2
14  [,14]   x.ege    mean edge count left to right
15  [,15]   xegvy    correlation of x.ege with y
16  [,16]   y.ege    mean edge count bottom to top
17  [,17]   yegvx    correlation of y.ege with x
```

P. W. Frey and D. J. Slate (Machine Learning Vol 6/2 March 91): "Letter Recognition Using Holland-style Adaptive Classifiers".

Example: Random Forest Code (build many simple models from subsets, use model averaging to predict)

Serial Code 4_rf_s.r

```
1  library(randomForest)
2  library(mlbench)
3  data(LetterRecognition) # 26 Capital Letters Data 20,000 x 17
4  set.seed(seed=123)
5  n <- nrow(LetterRecognition)
6  n_test <- floor(0.2*n)
7  i_test <- sample.int(n, n_test) # Use 1/5 of the data to test
8  train <- LetterRecognition[-i_test, ]
9  test <- LetterRecognition[i_test, ]
10
11 ## train random forest
12 rf.all <- randomForest(lettr ~ ., train, ntree=500, norm.votes=FALSE)
13
14 ## predict test data
15 pred <- predict(rf.all, test)
16 correct <- sum(pred == test$lettr)
17 cat("Proportion Correct:", correct/(n_test), "\n")
```

Example: Random Forest Code
(Split learning by blocks of trees. Split prediction by blocks of rows.)

Parallel Code 4_rf_p.r

```
1  library(randomForest)
2  library(mlbench)
3  data(LetterRecognition)
4  comm.set.seed(seed=123, diff=FALSE) # same training data
5  n <- nrow(LetterRecognition)
6  n_test <- floor(0.2*n)
7  i_test <- sample.int(n, n_test) # Use 1/5 of the data to test
8  train <- LetterRecognition[-i_test, ]
9  test <- LetterRecognition[i_test, ][get.jid(n_test), ]
10
11 comm.set.seed(seed=1e6*runif(1), diff=TRUE)
12 my.rf <- randomForest(lettr ~ ., train, ntree=500%/%comm.size(), norm.votes=FALSE)
13 rf.all <- do.call(combine, allgather(my.rf))
14
15 pred <- predict(rf.all, test)
16 correct <- allreduce(sum(pred == test$lettr))
17 comm.cat("Proportion Correct:", correct/(n_test), "\n")
```

Distributed Matrix and Vector Operations

A matrix is mapped to a processor grid shape

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

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

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

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

(a) 1×6 (b) 2×3 (c) 3×2 (d) 6×1

Table: Processor Grid Shapes with 6 Processors

Distributed Matrix and Vector Operations pbdDMAT

Powered by ScaLAPACK, PBLAS, and BLACS (MKL, SciLIB, or ACML)

- Block-cyclic data layout for scalability and efficiency
- No change in R syntax
- High-level convenience for data layout redistributions
  - Row-major data: read row-block then convert to block-cyclic
  - Column-major data: read column-block then convert to block-cyclic

Global and local views of block-cyclic on a 2×3 processor grid

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

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

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

pbdR No change in syntax. Data redistribution functions.

```
x <- x[-1, 2:5]
x <- log(abs(x) + 1)
x.pca <- prcomp(x)
xtx <- t(x) %*% x
ans <- svd(solve(xtx))
```

The above (and over 100 other functions) runs on 1 core with R or 10,000 cores with pbdR ddmatrix class

```
> showClass("ddmatrix")
Class "ddmatrix" [package "pbdDMAT"]
Slots:
Name:      Data      dim     ldim    bldim    ICTXT
Class:   matrix numeric numeric numeric numeric
```

```
> x <- as.rowblock(x)
> x <- as.colblock(x)
> x <- redistribute(x, bldim=c(8, 8), ICTXT = 0)
```

Truncated SVD from random projections[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: $\boldsymbol{B} = \widetilde{\boldsymbol{U}} \boldsymbol{\Sigma} \boldsymbol{V}^*$.
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

```
1  rSVD <- function(A, k, q=3)
2    {
3      ## Stage A
4      Omega <-  matrix(rnorm(n*2*k),
5          nrow=n, ncol=2*k)
6      Y <- A %*% Omega
7      Q <- qr.Q(qr(Y))
8      At <- t(A)
9      for(i in 1:q)
10       {
11         Y <- At %*% Q
12         Q <- qr.Q(qr(Y))
13         Y <- A %*% Q
14         Q <- qr.Q(qr(Y))
15       }
16
17     ## Stage B
18     B <- t(Q) %*% A
19     U <- La.svd(B)$u
20     U <- Q %*% U
21     U[, 1:k]
22   }
```

[1] Halko, Martinsson, and Tropp. 2011. Finding structure with randomness: probabilistic algorithms for constructing approximate matrix decompositions *SIAM Review* **53** 217–288

Truncated SVD from random projections

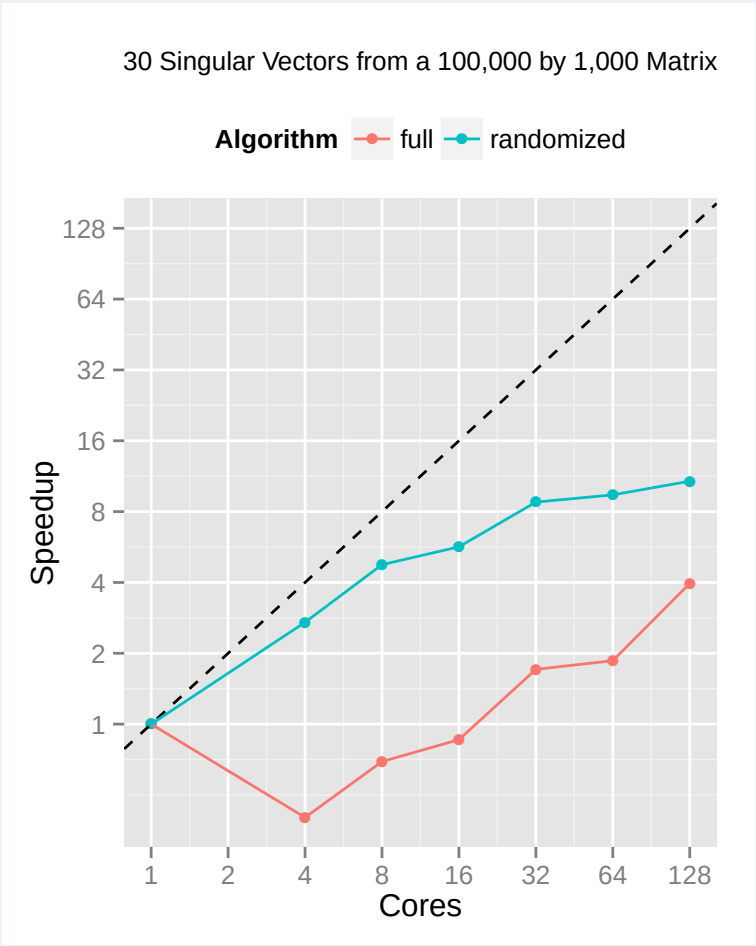
Serial R

```
1  rSVD <- function(A, k, q=3)
2    {
3      ## Stage A
4      Omega <- matrix(rnorm(n*2*k),
           nrow=n, ncol=2*k)
5      Y <- A %*% Omega
6      Q <- qr.Q(qr(Y))
7      At <- t(A)
8      for(i in 1:q)
9        {
10         Y <- At %*% Q
11         Q <- qr.Q(qr(Y))
12         Y <- A %*% Q
13         Q <- qr.Q(qr(Y))
14       }
15
16     ## Stage B
17     B <- t(Q) %*% A
18     U <- La.svd(B)$u
19     U <- Q %*% U
20     U[, 1:k]
21   }
```

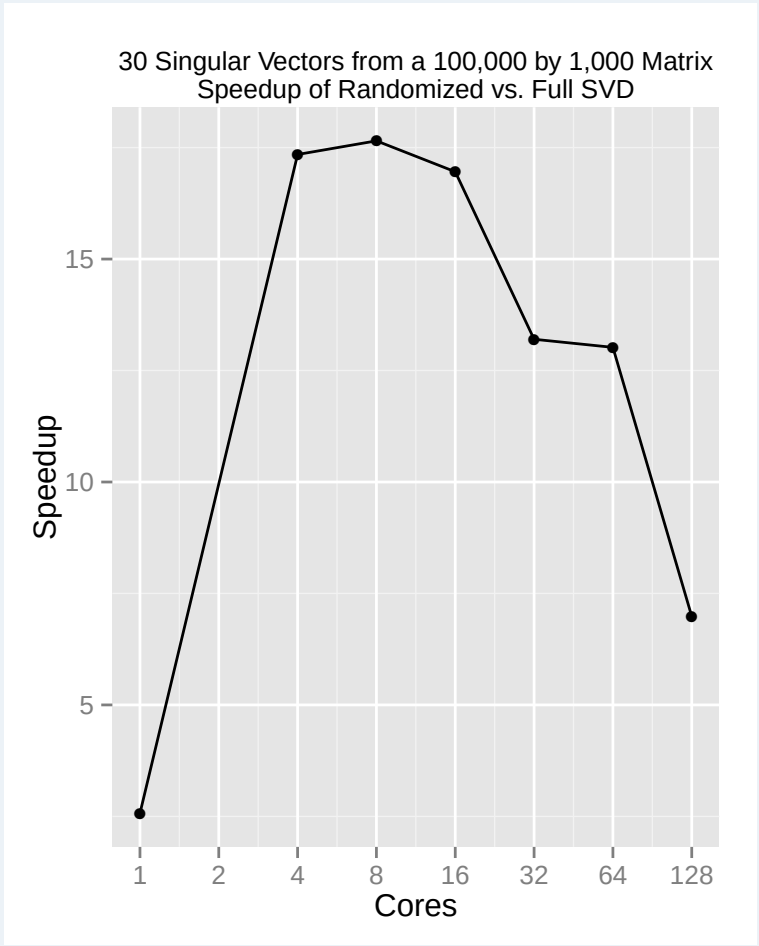
Parallel pbdR

```
1  rSVD <- function(A, k, q=3)
2    {
3      ## Stage A
4      Omega <- ddmatrix("rnorm",
5          nrow=n, ncol=2*k)
6      Y <- A %*% Omega
7      Q <- qr.Q(qr(Y))
8      At <- t(A)
9      for(i in 1:q)
10       {
11         Y <- At %*% Q
12         Q <- qr.Q(qr(Y))
13         Y <- A %*% Q
14         Q <- qr.Q(qr(Y))
15       }
16
17     ## Stage B
18     B <- t(Q) %*% A
19     U <- La.svd(B)$u
20     U <- Q %*% U
21     U[, 1:k]
22   }
```

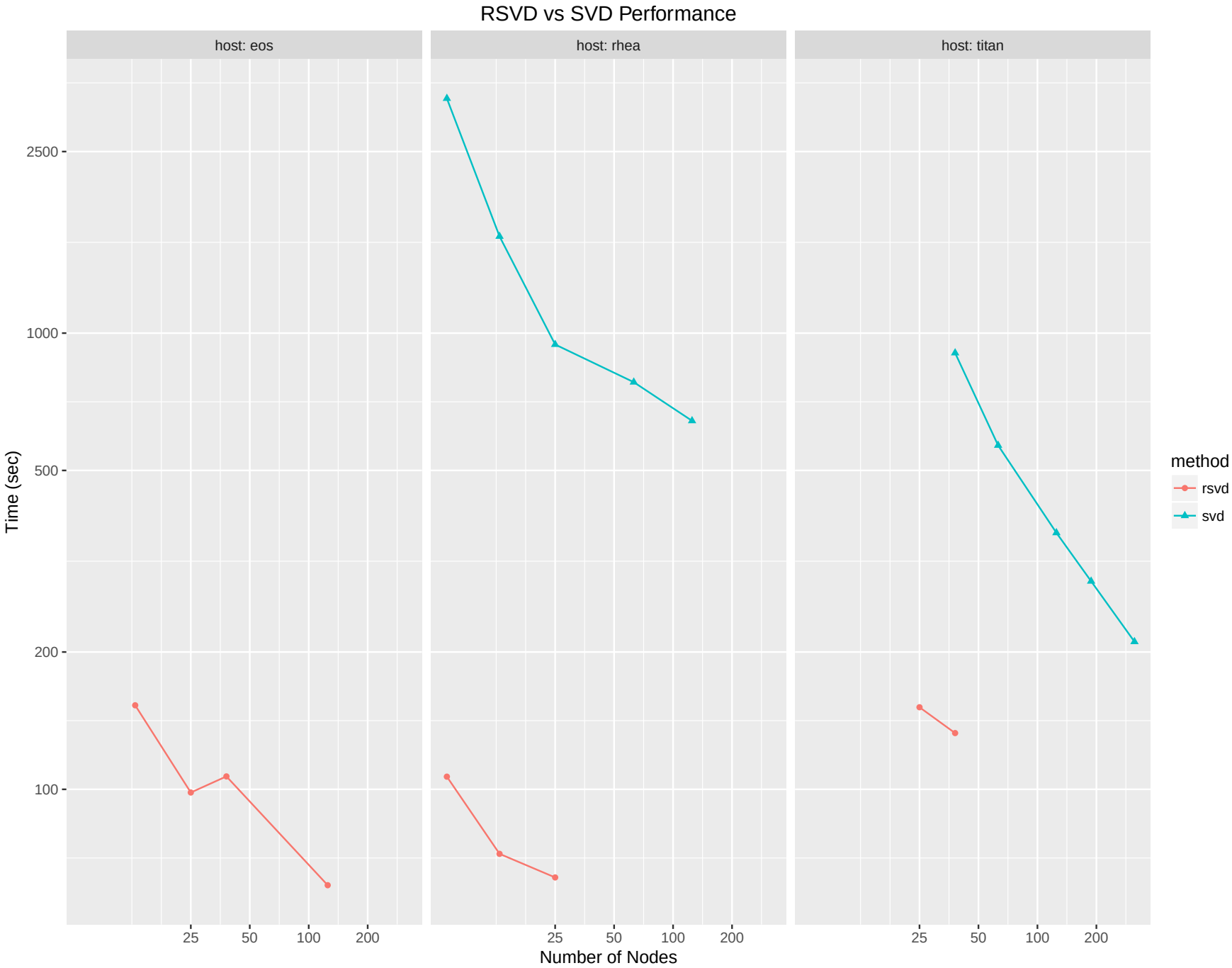
From journal to scalable code and scaling data in one day.

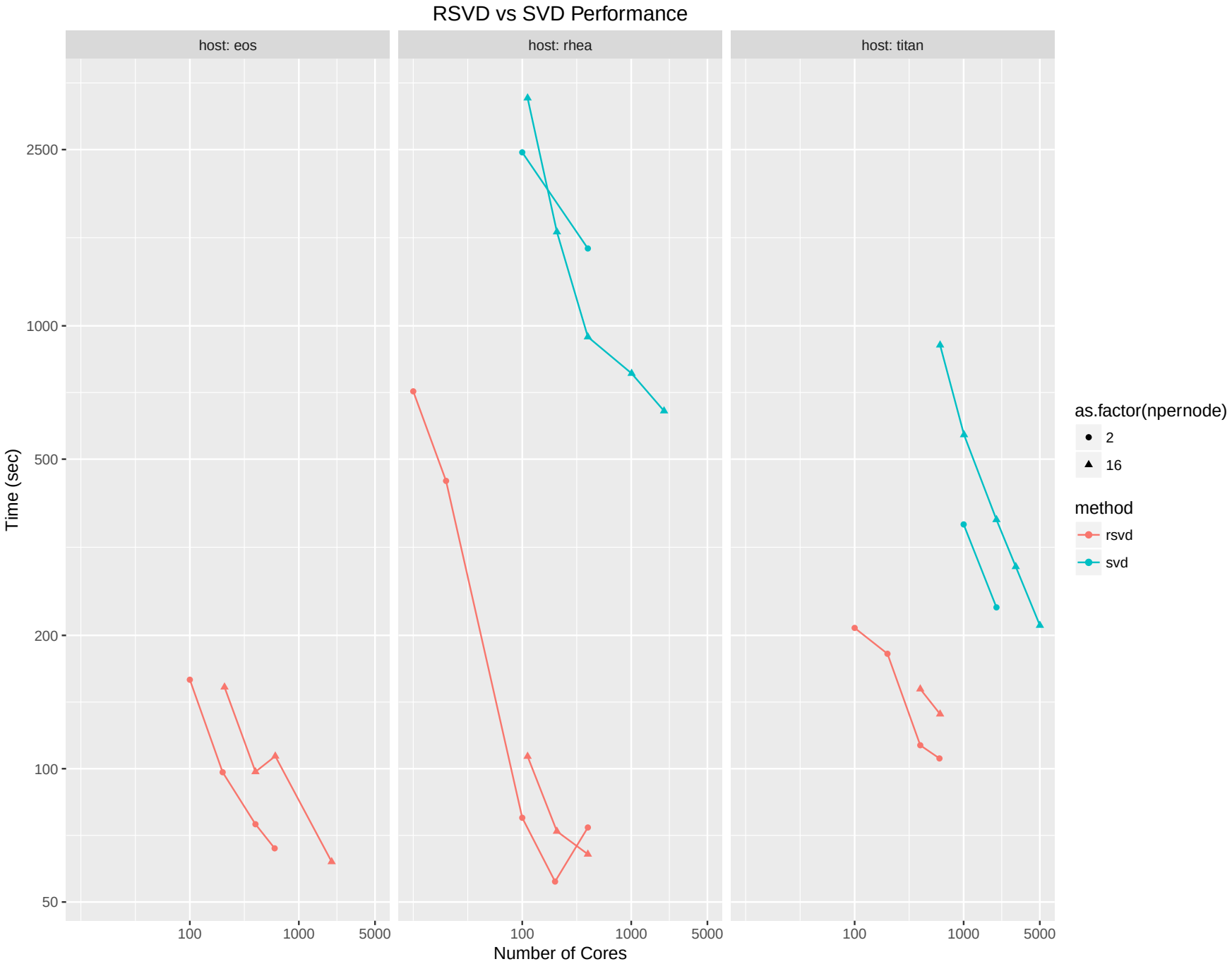


Speedup relative to 1 core



rSVD speedup relative to full SVD


RSVD vs SVD Performance
host: eos
host: rhea
host: titan
Time (sec)
2500
1000
500
200
100
25
50
100
200
Number of Nodes
method
rsvd
svd


RSVD vs SVD Performance
host: eos
host: rhea
host: titan
Time (sec)
2500
1000
500
200
100
50
100
1000
5000
Number of Cores
as.factor(npernode)
2
16
method
rsvd
svd

```
1  suppressMessages( library(rhdf5) )
2  suppressMessages( library(pbdDMAT, quiet=TRUE ) )
3  suppressMessages( library(pbdML, quiet=TRUE ) )
4
5  start.time = Sys.time( )
6  init.grid( )
7  end.time = Sys.time( )
8  barrier( )
9  comm.print( paste( "initgrid = ", end.time - start.time ) )
10
11 args = commandArgs( trailingOnly = TRUE )
12
13 meth      = args[ 1 ]
14 npernode  = strtoi( args[ 2 ] )
15 n_keep    = strtoi( args[ 3 ] )
16 block_row = strtoi( args[ 4 ] )
17 block_col = strtoi( args[ 5 ] )
18
19 nproc <- comm.size( )
20
21 rows <- 12390000 %/% nproc
22 cols <- 1250
23
24 len <- rows*cols*4
25 start <- comm.rank()*len
26
27 ## this one has individual files
28
29 if ( nproc ==     2 ) fn <- paste("X/X2", comm.rank(), "h5", sep=".")
30 if ( nproc ==     4 ) fn <- paste("X/X4", comm.rank(), "h5", sep=".")
31 if ( nproc ==     5 ) fn <- paste("X/X5", comm.rank(), "h5", sep=".")
32 if ( nproc ==    10 ) fn <- paste("X/X10", comm.rank(), "h5", sep=".")
33 if ( nproc ==    20 ) fn <- paste("X/X20", comm.rank(), "h5", sep=".")
34 if ( nproc ==   100 ) fn <- paste("X/X100", comm.rank(), "h5", sep=".")
35 if ( nproc ==   200 ) fn <- paste("X/X200", comm.rank(), "h5", sep=".")
```

```
36 if ( nproc ==   400 ) fn <- paste("X/X400", comm.rank(), "h5", sep=".")
37 if ( nproc ==   600 ) fn <- paste("X/X600", comm.rank(), "h5", sep=".")
38 if ( nproc ==  1000 ) fn <- paste("X/X1000", comm.rank(), "h5", sep=".")
39 if ( nproc ==  2000 ) fn <- paste("X3/X2000", comm.rank(), "h5", sep=".")
40 if ( nproc ==  3000 ) fn <- paste("X3/X3000", comm.rank(), "h5", sep=".")
41 if ( nproc ==  5000 ) fn <- paste("X5/X5000", comm.rank(), "h5", sep=".")
42 if ( nproc == 30000 ) fn <- paste("X/X30000", comm.rank(), "h5", sep=".")
43
44 start.time = Sys.time( )
45 A <- h5read(fn, "/dataset" )
46 end.time = Sys.time( )
47 barrier( )
48 comm.print( paste( "io = ", end.time - start.time ) )
49
50 ## comm.print( A[ 1:5, 1:5 ], all.rank = TRUE )
51 ## comm.print( dim( A ), all.rank = TRUE )
52 start.time = Sys.time( )
53 A <- new( "ddmatrix", Data=A, dim=c(12390000, 1250), ldim=dim(A), bldim=dim(A),
       ICTXT=2 )
54
55 ## comm.print( dim(submatrix( A )), all.rank = TRUE )
56 ## comm.print( submatrix( A )[ 1:5, 1:5 ], all.rank = TRUE )
57 ## comm.print( A, all.rank = TRUE )
58
59 A <- as.blockcyclic( A, bldim = c( block_row, block_col ) )
60
61 ## comm.print( A[ 1:5, 1:5 ], all.rank = TRUE )
62 ## comm.print( dim( A ), all.rank = TRUE )
63
64 end.time = Sys.time( )
65 barrier( )
66 comm.print( paste( "blockcyclic = ", end.time - start.time ) )
67
68 ## comm.print( A, all.rank = TRUE )
69 ## comm.print( submatrix( A )[ 1:5, 1:5 ], all.rank = TRUE )
```

```
70   comm.print( "Starting computation" )
71  start.time = Sys.time( )
72  if ( meth == "rsvd" )
73    Res <- rsvd( A, k = n_keep, q = 3, retu = TRUE, retv = TRUE )
74  if ( meth == "gpu_rsvd" )
75    Res <- rsvd( A, k = n_keep, q = 3, retu = TRUE, retv = TRUE )
76  if ( meth == "gpu_svd" )
77    Res <- svd( A, nu = n_keep, nv = n_keep )
78  if ( meth == "svd" )
79    Res <- svd( A, nu = n_keep, nv = n_keep )
80  end.time = Sys.time( )
81  barrier( )
82  comm.print( paste( "compute = ", end.time - start.time ) )
83
84  comm.print( Res$d )
85  mesg <- paste( "Finished ... method =", meth, "nproc =", nproc, "npernode =",
        npernode, "keep =", n_keep, "blocking =", block_row )
86  comm.print( mesg )
87
88  finalize( )
```

Where to learn more?

- http://r-pbd.org/
- **pbdDEMO** vignette
- Googlegroup:RBigDataProgramming
- pbdR Installations: OLCF, NERSC, SDSC, TACC, IU, BSC Spain, CSCS Switzerland, IT4I Czech, ISM Japan, and many more

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