The pbdR Project: Distributed Computing with R*

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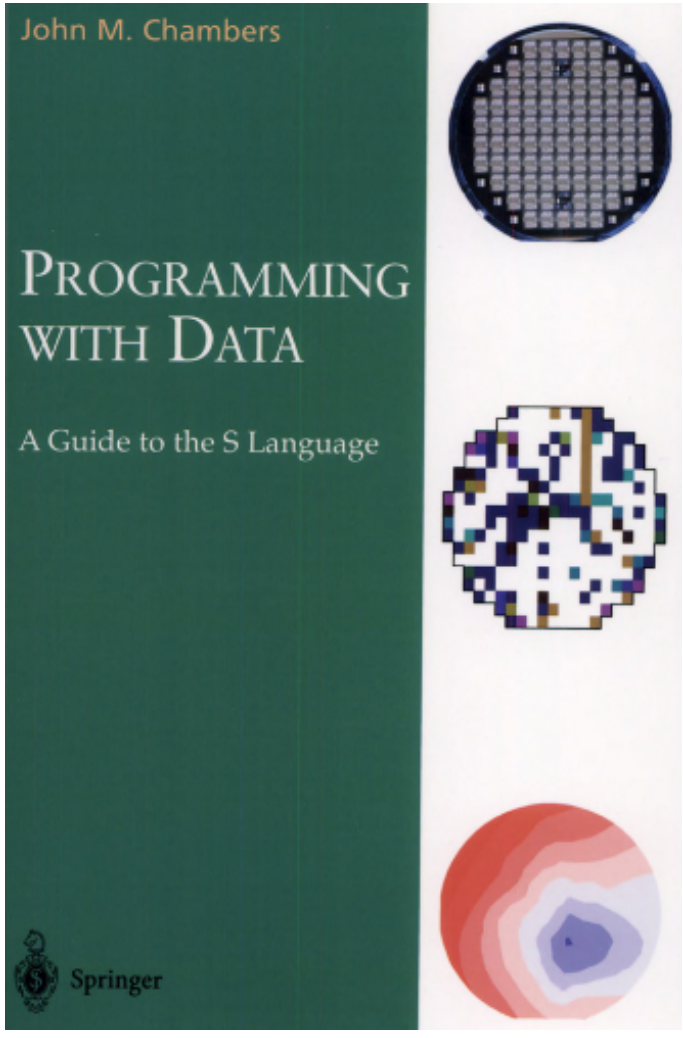
Outline

What is pbdR

- Around 1998, a book "*Programming with Data – A Guide to the S Language*" by John M. Chambers was published.
- Around 2012, the "**P**rogramming with **B**ig **D**ata in **R**" project was started with a set of highly scalable R packages for distributed computing and profiling in data science.

pbdR
Programming with Big Data in R



Where to learn pbdR

- Main website:
  - http://pbdr.org/
- Main release:
  - http://pbdr.org/release/
- Main repository:
  - https://github.com/RBigData/
- Where to start:
  - pbdDEMO vignettes (about 150 pages) at `https://cran.r-project.org/web/packages/pbdDEMO/vignettes/pbdDEMO-guide.pdf`
  - pbdMPI vignettes (about 30 pages) at `https://cran.r-project.org/web/packages/pbdMPI/vignettes/pbdMPI-guide.pdf`

How can pbdR help?

- Performance, performance, performance ...

Parallel pbdR

```
1  randSVD <- function(A, k, q=3)
2    {
3      ## Stage A
4      Omega <- ddmatrix("rnorm", 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   }
```

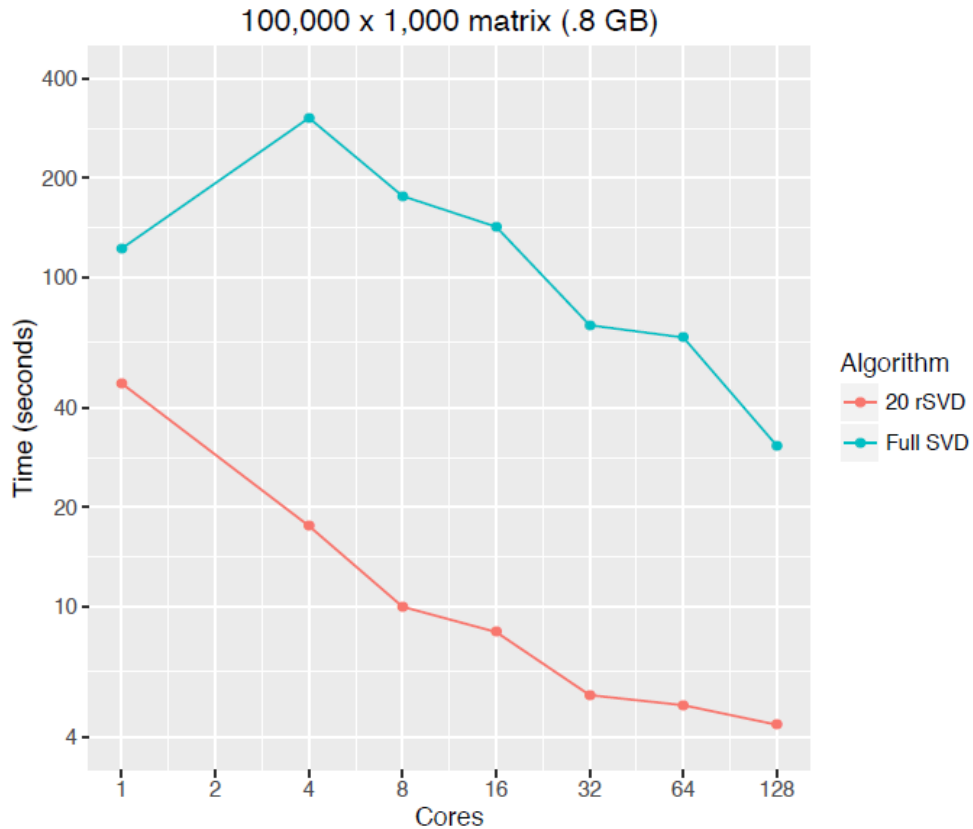


Figure 1: Parallelizing the function by one line. Execute the function in any # of cores. Obtain the results faster.

Illustration of Parallelism

- Popular for statistical simulations
- Efficient for small size of data or dividable data/tasks

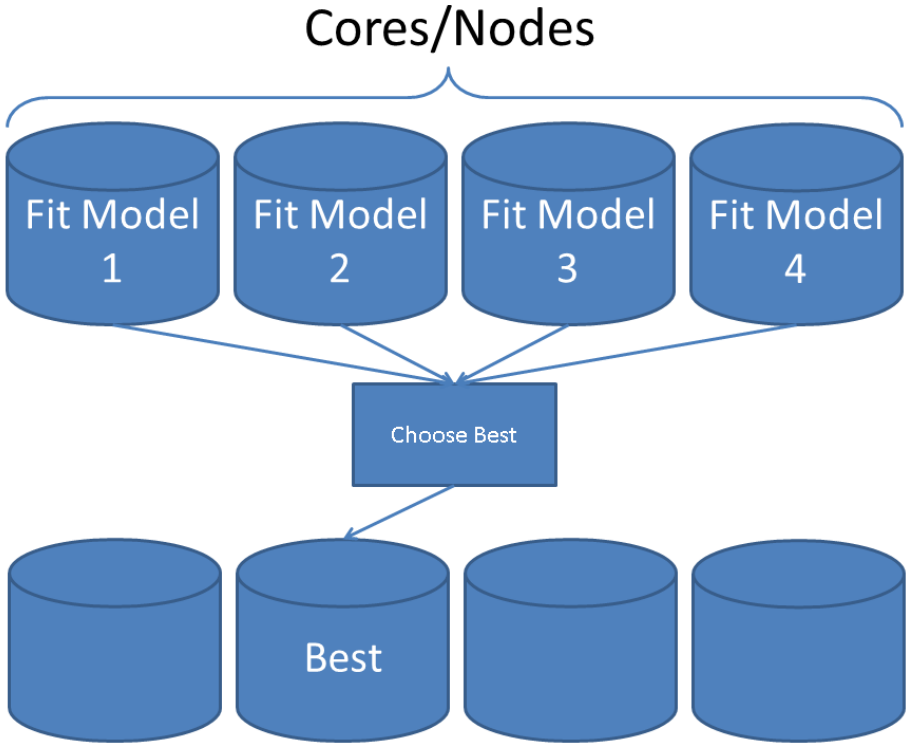


Figure 2: Task Parallelism

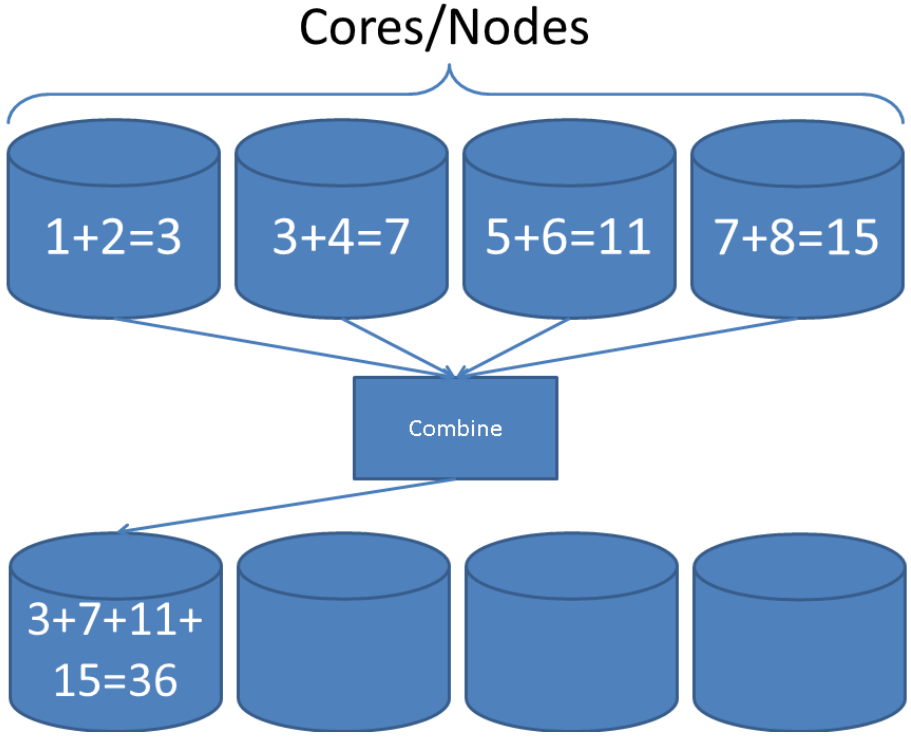


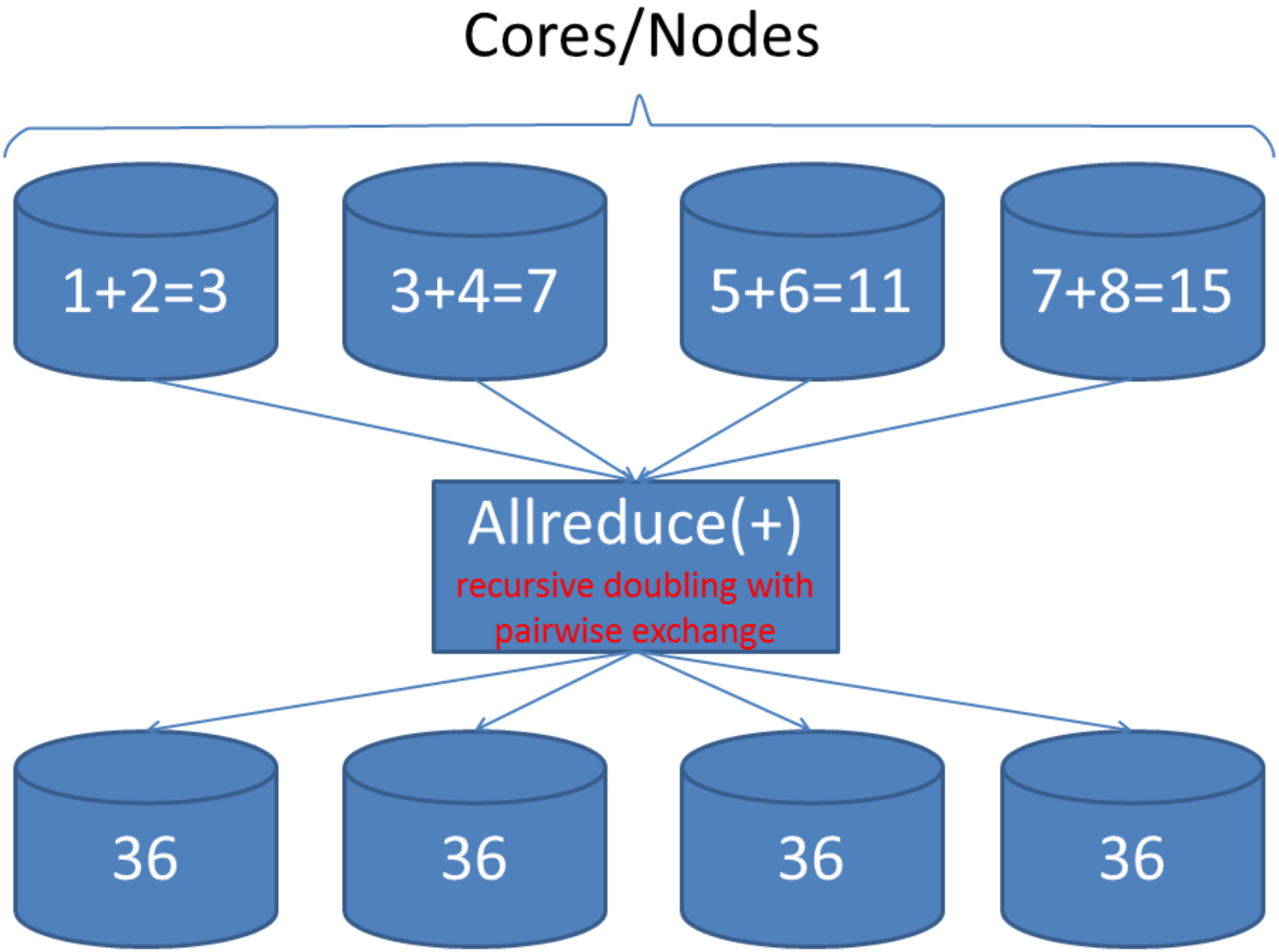
Figure 3: Data Parallelism

SPMD & MPI

SPMD in Wikipedia:
... In computing, SPMD (single program, multiple data) is a technique employed to achieve parallelism; ... *Tasks are split up and run simultaneously on multiple processors with different input in order to obtain results faster.* SPMD is the most common style of parallel programming ... *The current de facto standard is MPI* ...

MPI in Wikipedia:
Message Passing Interface (MPI) is a standardized and portable message-passing standard ... to function on a wide variety of parallel computing architectures... Language bindings R bindings of MPI include Rmpi and pbdMPI where Rmpi focuses on manager-workers parallelism while *pbdMPI focuses on SPMD parallelism*...

An SPMD Example



The Power of MPI Reduction Operations

$$X = \begin{pmatrix} X_0 \\ \vdots \\ X_7 \end{pmatrix} \text{ then } X^T X = \sum_{i=0}^{7} X_i^T X_i$$

```
Library(pbdMPI)
myrank = comm.rank()

## construct a matrix chunk
X = matrix(100*myrank + 1:8, nrow=4)

XtXloc = crossprod(X)

XtX = allreduce(XtXloc)

## everyone has XtX

finalize()
```

SPMD

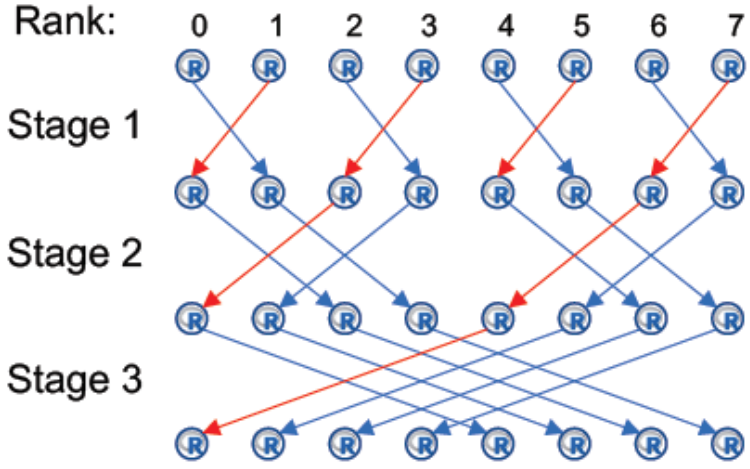
```
> myrank
[1] 0
> X
     [,1] [,2]
[1,]    1    5
[2,]    2    6
[3,]    3    7
[4,]    4    8
```

```
> myrank
[1] 7
> X
     [,1] [,2]
[1,]  701  705
[2,]  702  706
[3,]  703  707
[4,]  704  708
```

```
> XtX
         [,1]    [,2]
[1,] 5656240 5701360
[2,] 5701360 5746992
```

Recursive doubling with pairwise exchange

allreduce(), reduce(), allgather(), gather()



Communication stages when reduction is associative		
Processors	MapReduce shuffle	MPI allreduce
8	**7**	**3**
128	**127**	**8**
n	**n - 1**	**$\log_2 n$**

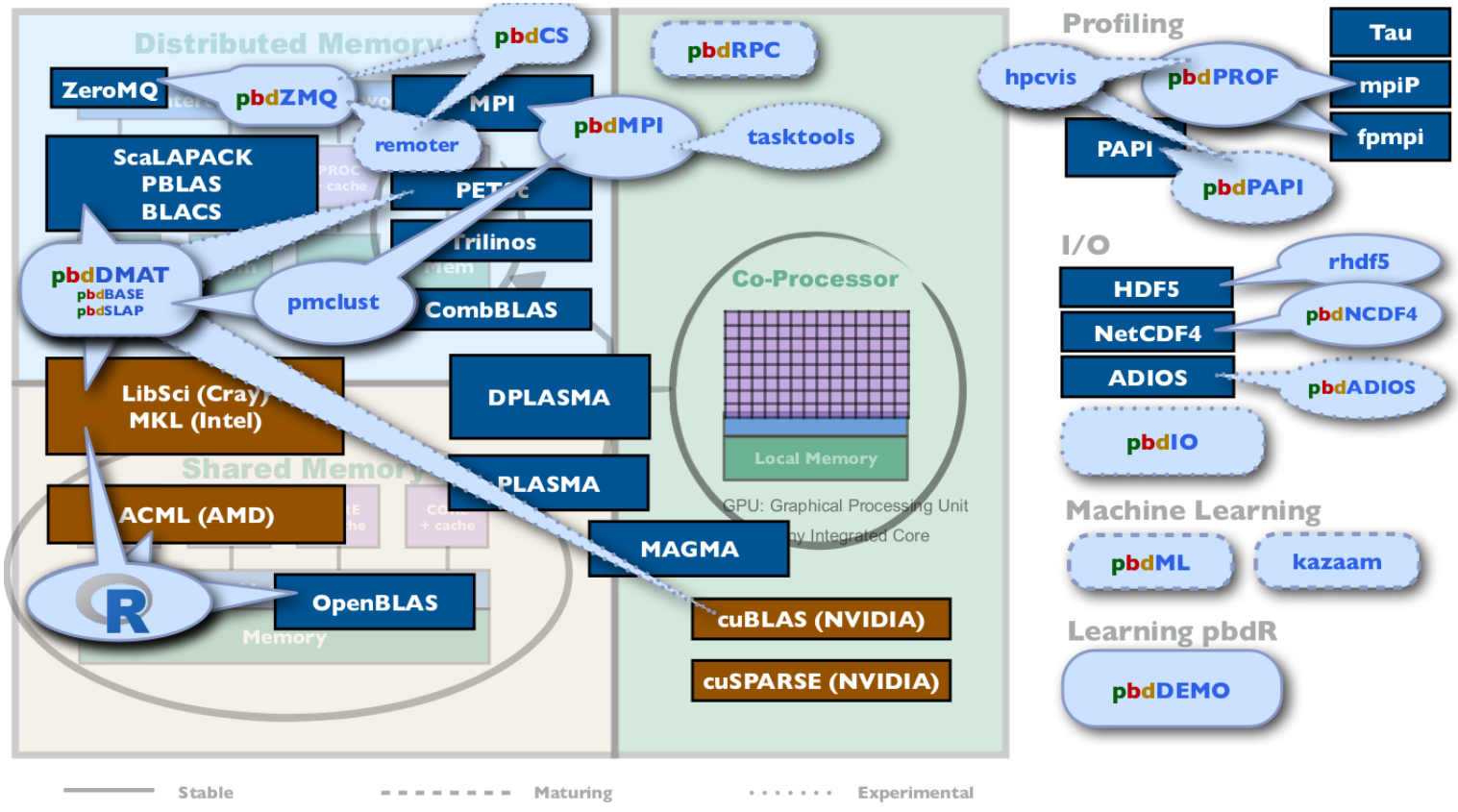
pbdR Thinking

Strive for *Productivity, Portability, Performance*

- Bridge high-performance computing with high-productivity of R language
- Keep syntax *identical* to native R , when possible
- Software reuse philosophy:
  - Don't reinvent the wheel when possible
  - Introduce HPC standards with R flavor
  - Use scalable HPC libraries with R convenience
- Simplify and use R intelligence where possible

pbdR v1.0-1 (Apr 2018) at `http://pbdr.org/releases/`

- MPI packages: pbdMPI, pbdSLAP, pbdBASE, pbdDMAT, kazaam, tasktools
- Statistical Applications: pbdML, pmclust, pbdDEMO
- Communication tools: pbdZMQ, remoter, pbdCS, pbdRPC
- Profilers: pbdPROF, pbdPAPI, hpcvis
- I/O packages: pbdIO, pbdNCDF4, pbdADIOS, hdfio



Dense Distributed Linear Algebra and Statistics

See vignettes of pbdBASE, pbdDMAT, and kazaam.

- pbdBASE and pbdDMAT provides block or block-cyclic distributed matrices, algebra, and operations.

- kazaam is designed for "tall but skinny" matrices where data are distributed in row blocks.

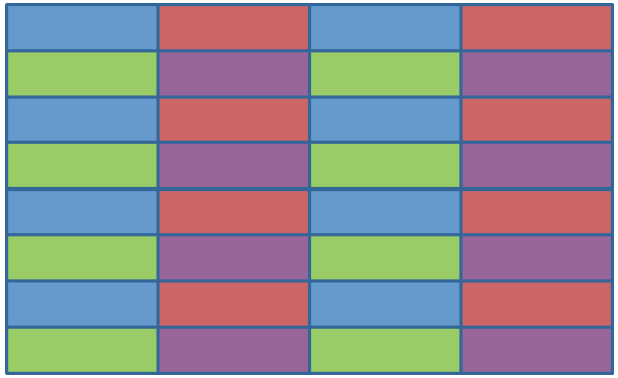


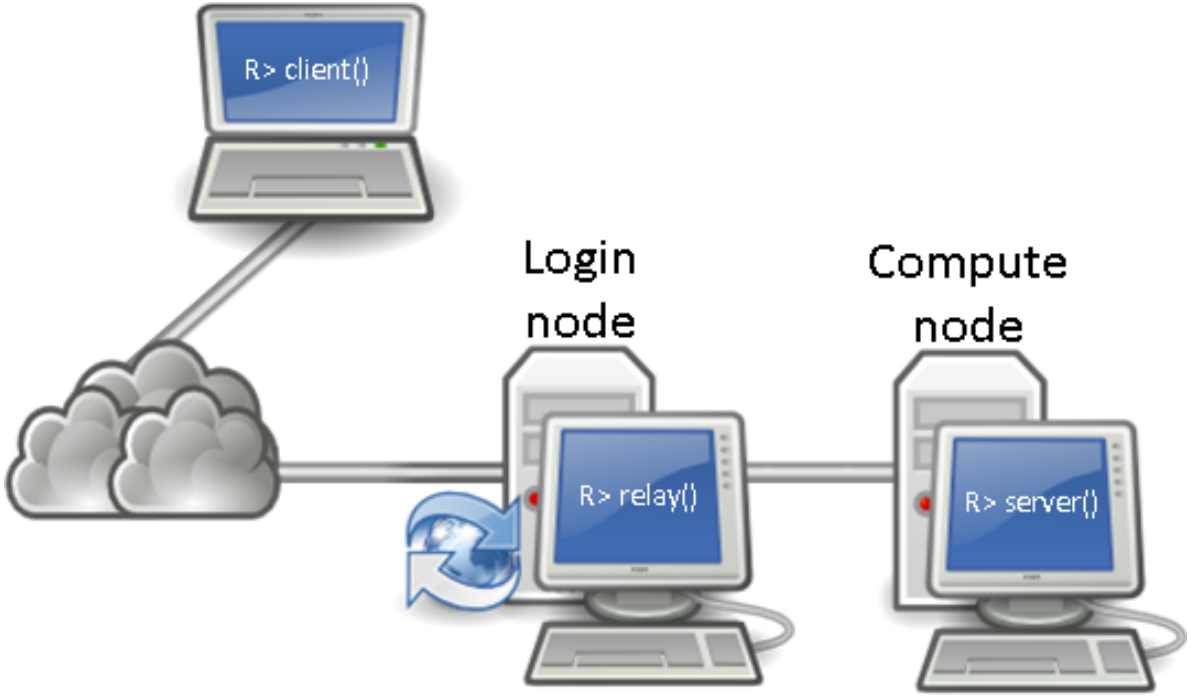
Figure 4: A 2D block cyclic matrix distributed in 4 cores (indicated by colors).

Figure 5: A tall but skinny matrix distributed in 4 cores (indicated by colors).

Client Server(s) in SPMD

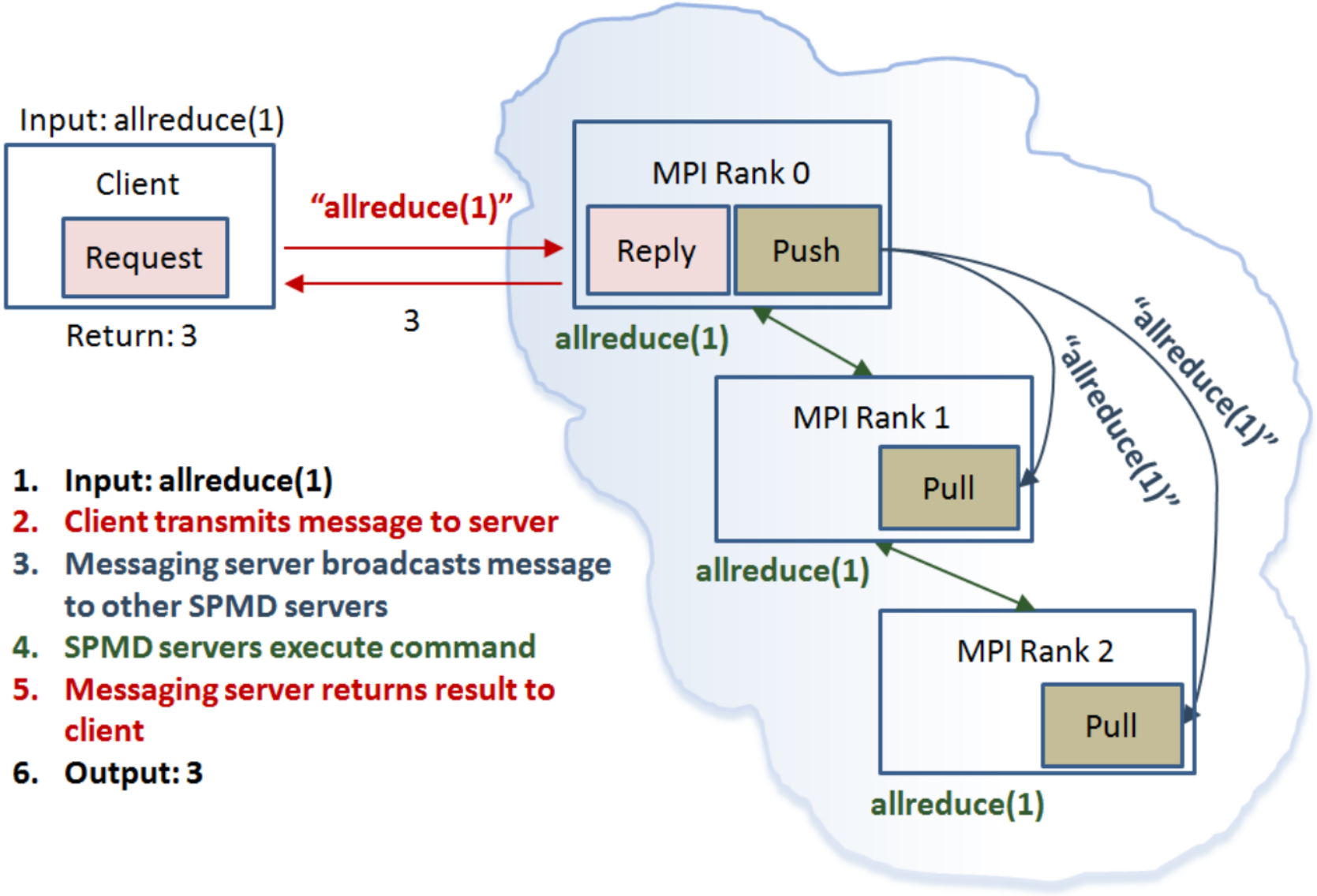
See demos at
https://github.com/snoweye/user2016.demo

- remoter + pbdZMQ: one client and one server
- pbdCS + remoter + pbdZMQ: one client and many MPI/SPMD servers, clusters, or HPC computing nodes
- pbdRPC: remote procedure calls to start the server(s)

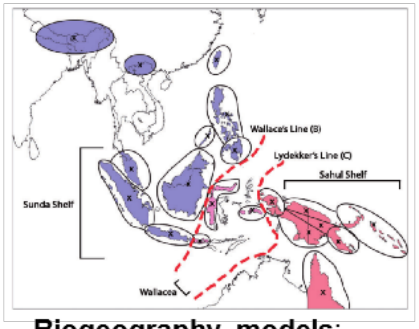


Basic Interaction with SPMD

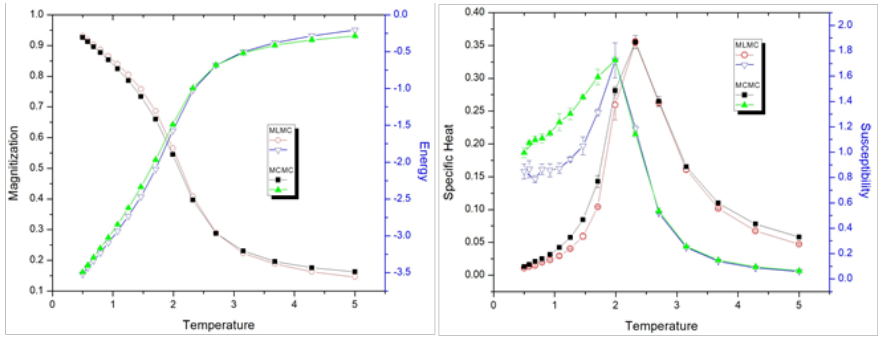
- Big data are obtained by and stays distributed on the servers
- The client sends only code to the server executing in SPMD



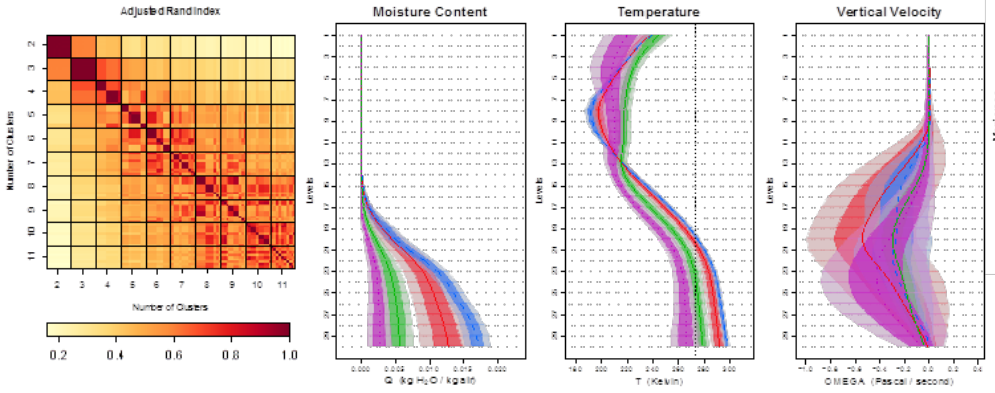
Diverse Statistical Applications of pbdR Analytics



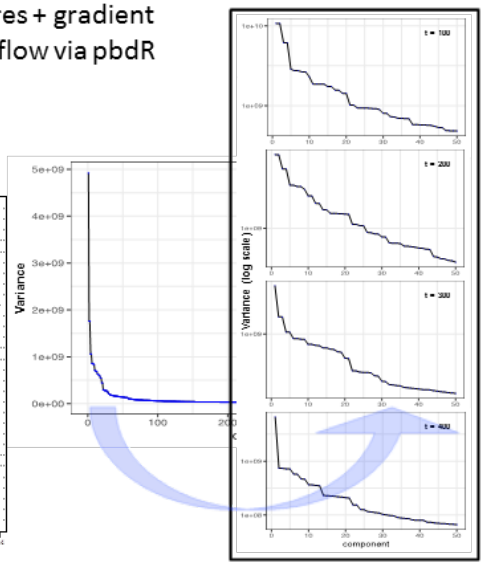
Biogeography models: distributed matrix exponentials (*UseR, 2014*)

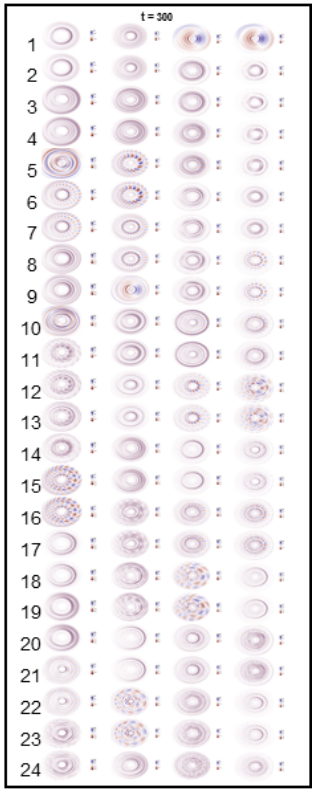


MCMC DFT: Deep neural network features + gradient boosting surrogate model. Parallel workflow via pbdR (*CoDA 2018*)



Climate extremes extraction and clustering with mixture models: scalable graphics, Rand index uncertainty, 3 TB data (*Technometrics, 2013*)





Fusion simulation: extracting coherent turbulence structures (*CoDA 2018*)

Statistical Algorithms and Methods

All algorithms and methods are in SPMD (i.e. parallel and distributed). Again, see pbdDEMO vignettes for more.

- Implemented:
  - matrix/vector operations, matrix decompositions, summary statistics, random number generation
  - pbdDMAT: linear model, logistic regression, SVM
  - kazaam: k-means, linear model, glm fitters (Gaussian, Logistic, Poisson)
  - pmclust: k-means, model-based clustering, EM/APECM algorithms
  - pbdML: random SVD/PCA, robust PCA, Fisher's linear discriminant
- Future plan:
  - pbdML: SVM, random forest, neural network, bagging, boosting, etc
  - *How about yours?!*

Computational Statistics Utilities

The tasktools is designed for task-based parallelism which is especially useful for multiple but independent simulations, MCMC, long searching for optimal study design.

- Include an lapply()-like interface
- More convenient than pbdMPI::pbdLapply() or Rmpi
- Automatically handles input-checkpointing:
  - Have thousands of ”jobs”
  - Run as many as you can in 2 hour run window
  - Keep running job until all tasks eventually complete
- Can be used as a workflow tool for external programs

Extensions to Data Science

User interfaces (R packages) developed by external groups that rely on pbdR (mainly pbdZMQ):

- IRkernel: Native R Kernel for the 'Jupyter Notebook' at `https://github.com/IRkernel/IRkernel`
- JuniperKernel: Kernel for 'Jupyter' at `https://github.com/JuniperKernel/JuniperKernel`

Summary

- Engage parallel math libraries at scale
- R language unchanged
- New distributed concepts
- New interactive SPMD parallel
- Broad analysis and statistical applications

Not included in this talk:

- New profiling capabilities
- Parallel and high performance I/O
- Comparisons with other frameworks:
  - A review paper: Thomas & Kumar (2018) “A Comparative Evaluation of Systems for Scalable Linear Algebra-based Analytics.”
  - From HPC wire, July 6, 2016: “OLCF Researchers Scale R to Tackle Big Science Data Sets” ... “**for ... interactive near-real-time analysis, the pbdR approach is much better** [than Apache Sparklike frameworks]. PCA of a 134 GB matrix: “hours on ... Apache Spark, ... less than a minute using R.”

Acknowledgement

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Thank you!