

Statistical Computing on Large Parallel Architectures

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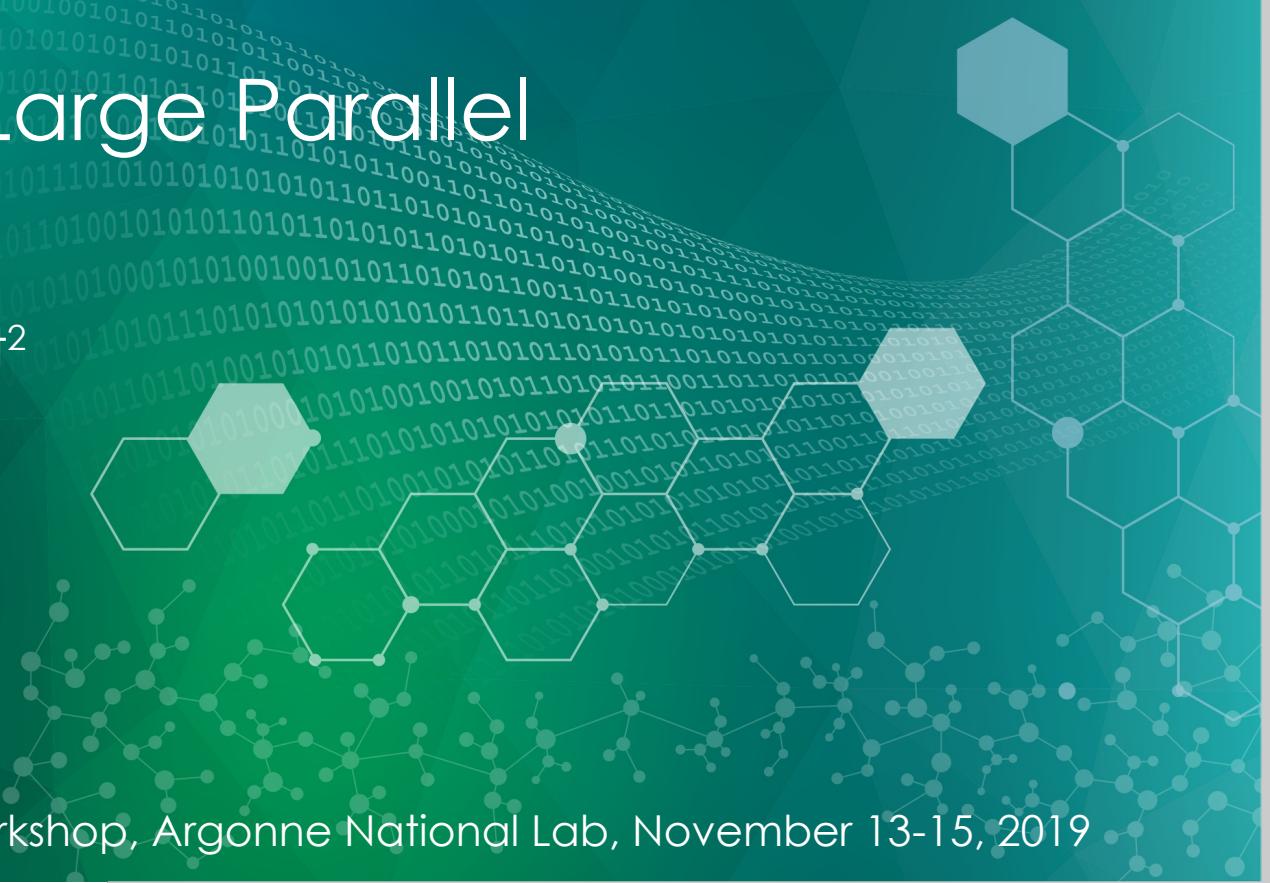
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Advanced Statistics meets Machine Learning III Workshop, Argonne National Lab, November 13-15, 2019

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Statistics is to Machine Learning
as Physics is to Engineering

Physical Sciences

- Mathematics
- Physics
- Engineering

ABSTRACTION

IMPLEMENTATION

Data Sciences

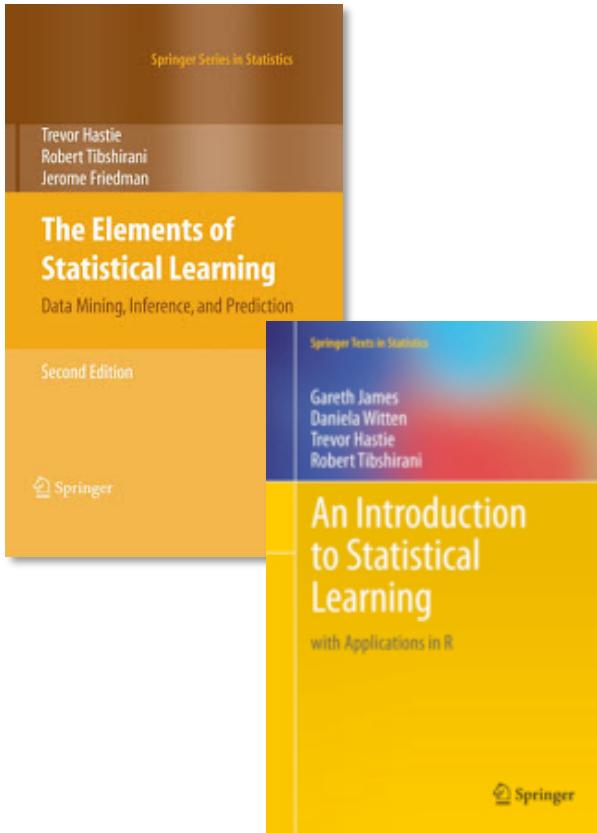
- Mathematics
- Statistics
- Machine Learning

Statistics is the “Physics” of Data

Machine Learning or Statistical Learning?

Both are about **learning from data**, some difference in emphasis:

- SL: Explainability and discovery, uncertainty is fundamental
- ML: Processing and prediction, uncertainty is optional

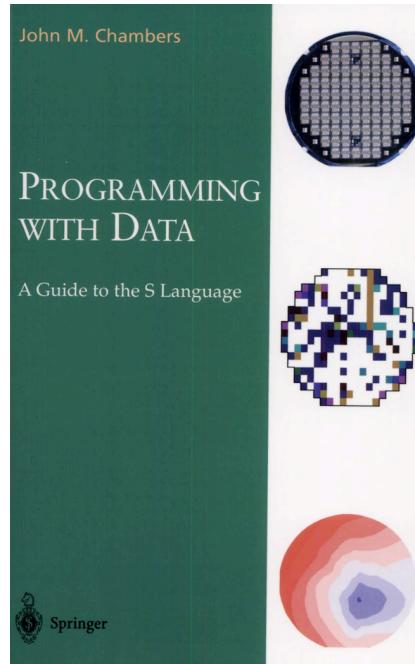


Dictionary

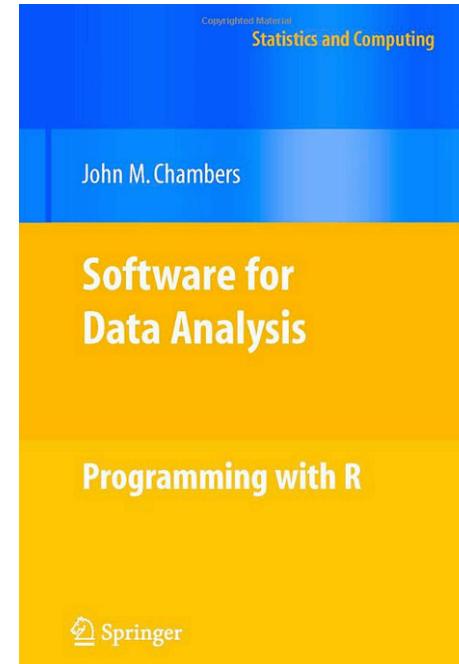
Machine Learning	Statistical Learning
Accuracy	(lack of) Bias
Bias	Intercept
Generalization	Test set performance or Expected prediction error
Inference	Prediction, point estimate
Learning	Fitting
Network, graph	Model
One-hot	Dummy variable
Precision	(lack of) Variability
Supervised learning	Regression/classification
Uncertainty	Inference
Unsupervised learning	Density estimation, clustering
Weights	Parameters

Adapted from Rob Tibshirani (Stanford) and expanded

Language for Programming with Data: R



1998 S language



2008 R language

Same language, different engine

2019 IEEE Spectrum's Ranking of Programming Languages

Rank	Language	Type	Score
1	Python	🌐💻⚙️	100.0
2	Java	🌐📱💻	96.3
3	C	📱💻⚙️	94.4
4	C++	📱💻⚙️	87.5
5	R	💻	81.5
6	JavaScript	🌐	79.4
7	C#	🌐📱💻⚙️	74.5
8	Matlab	💻	70.6
9	Swift	📱💻	69.1
10	Go	🌐💻	68.0

Diversity for Data and Depth for Statistics in R



Bringing Modern Statistical Science and R to HPC

Core Team (leadership and lead developers)

Wei-Chen Chen, US FDA

George Ostrouchov, ORNL & UTK

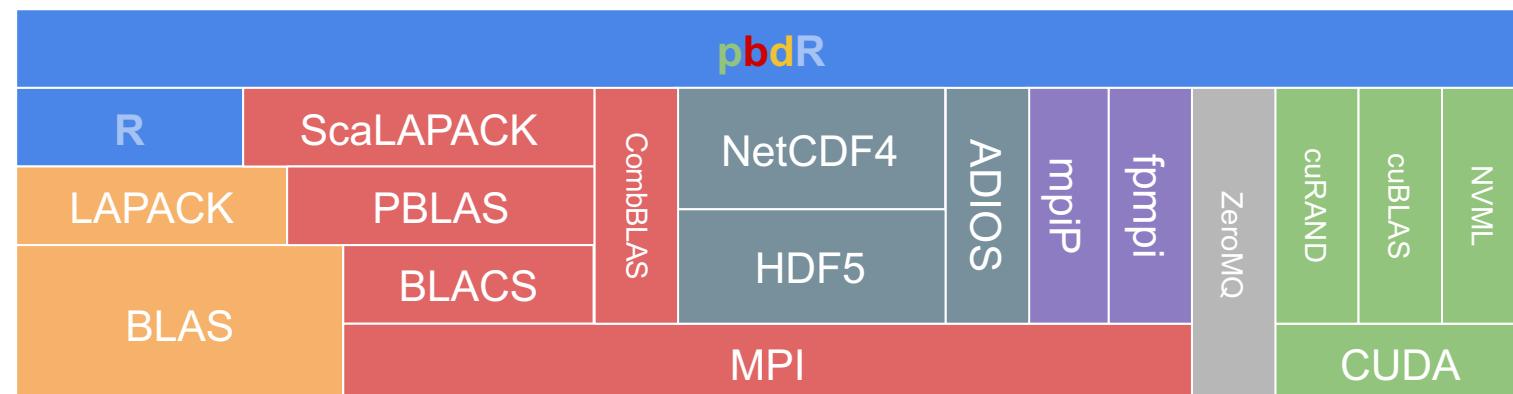
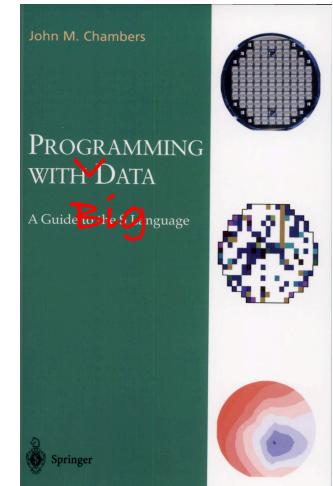
Drew Schmidt, ORNL

Developers

Christian Heckendorf, Yuping Lu, Michael Matheson, Pragneshkumar Patel, Gaurav Sehrawat , Amil Williamson

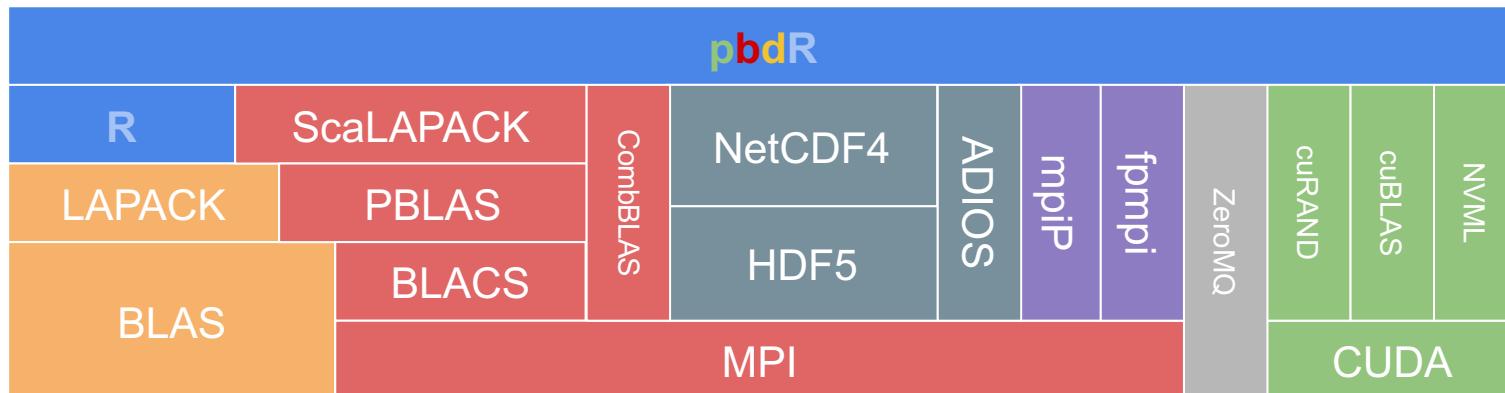
Contributors

Moustaffa Ahmed, Whit Armstrong, Ewan Higgs, Sébastien Lamy de la Chapelle, Michael Lawrence, Andrey Paul, A. Philipp, David Pierce, Brian Ripley, Elliott Sales, Aiello Spencer, ZhaoKang Wang, Hao Yu



pbdR Philosophy

- Bridge high-performance computing with high-productivity of R language
- Keep syntax *identical* to 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 ... outperformed all the other systems in almost all cases on dense data.”

“Overall, pbdR is best suited to users who want to rapidly prototype new LA-based analysis algorithms at scale”

- An independent comparison on small distributed systems with up to 8 nodes (224 cores)
- Software considered: **pbdR**, **MADlib**, **MLlib**, **SystemML**, and **TensorFlow**
- Computations considered: distributed analytics based on linear algebra

Anthony Thomas, Arun Kumar: [A Comparative Evaluation of Systems for Scalable Linear Algebra-based Analytics](#). *Proceedings of the VLDB Endowment*, Volume 11, No. 13, September 2018, p. 2168-2182.



Parallel I/O

- **hdfio**
 - High-level utilities for working with data frames in [HDF5](#) and sharing between Python and R
 - See [rhdf5](#) and [hdf5r](#) packages for lower level utilities
 - <https://code.ornl.gov/olcf-analytics/summit/r/blob/master/content/pbdR/hdfio.md>
- **pbdIO**
 - So far mostly for parallel reads of collections of CSV files
 - Chunking, data frame rebalancing
- **pbdADIOS**
 - ADIOS 1.8, can stream with in-memory files, needs development for transition to ADIOS 2.0.
- **pbdNCDF4**
 - NetCDF4 file collective parallel reads and writes
- **In situ capabilities**
 - Communicator management, in-memory streaming file reads

Advanced CPU Analytics

- Packages: `pbdDMAT` (and friends), `kazaam`, `pbdML`, `pmclust`, `pbdXGB`
 - k-means and Model-Based Clustering
 - GLM's
 - Fisher's Linear Discriminant
 - Randomized SVD/PCA, Robust PCA
 - Gradient Boosting Machines and Random Forests via XGBoost
- Parallel dense matrix and sparse matrix infrastructure for custom distributed methods

Striving for interactive performance on Terabyte-sized data analysis



July 6, 2016

"OLCF Researchers Scale R to Tackle Big Science Data Sets" . . . "for situations where one needs interactive near-real-time analysis, the pbdR approach is much better [than Apache Spark-like frameworks]."

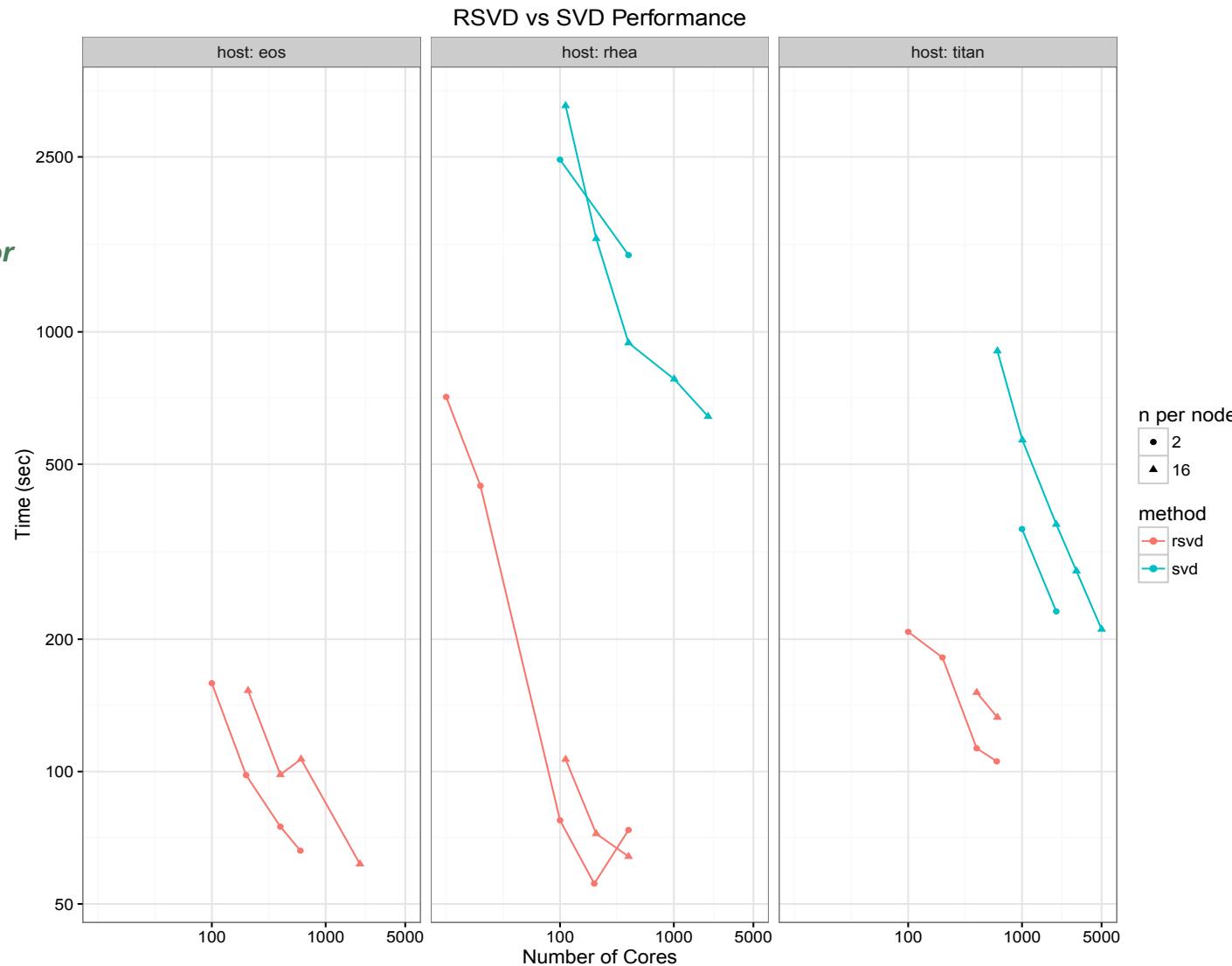
PCA of a 134 GB matrix: "hours on . . . Apache Spark, . . . less than a minute using R."

April 20, 2017

"ORNL Researchers Bridge the Gap Between R, HPC Communities" . . . "untapped [R] domains" represent an enormous potential user base for world-class computers ."

May 7, 2018

"ORNL Data Scientists Release pbdR 1.0"



Seconds for 150 TB SVM Computation on Half of Summit

GPU Analytics benchmarks

- Packages: **dimrgame**, **clustrgame**, **glmrgame**
 - SVM, SVD, PCA, k-means

Example code with small toy data (benchmark data is more complex)

```
suppressMessages(library(kazaam))
suppressMessages(library(glmrgame))

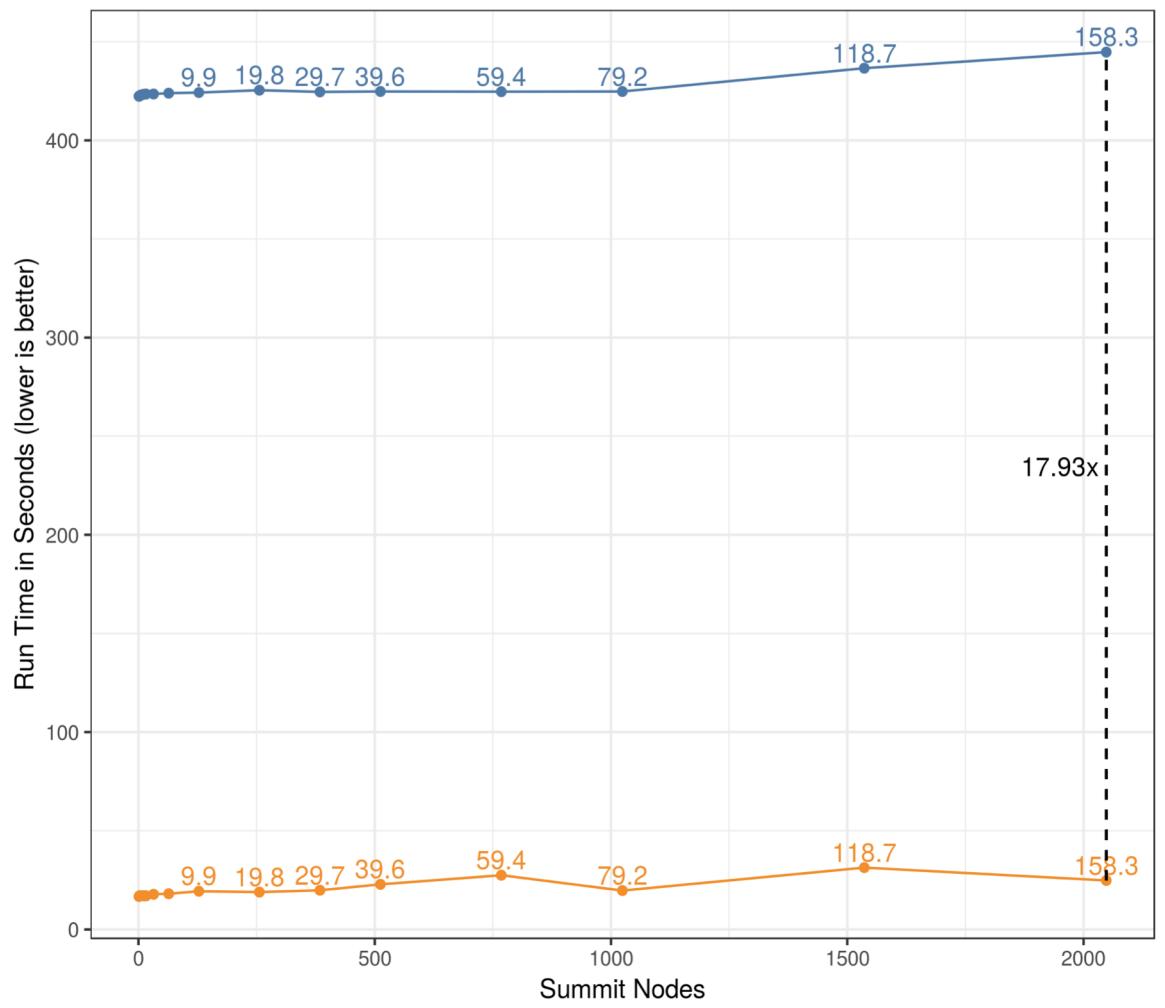
data(iris)
is_setosa = expand((iris[, 5] == "setosa")*2 - 1)
iris = expand(as.matrix(iris[, -5]))
iris = cbind(shaq(1, nrow=nrow(iris), ncol=1), iris)

w_cpu = svm(iris, is_setosa)
w_gpu = svm_game(iris, is_setosa)

finalize()
```

CORAL 2 SVM Weak Scaling Benchmark

Point labels are problem size in TB



Implementation ● cpu ● gpu

Low-Level GPU Tools

nvsmi

```
options("nvsmi_printer"="minimal")
nvsmi::smi()

## +-----+
## | Date: Thu Apr 18 12:44:24 2019          Driver Version: 390.116 |
## |-----+-----+-----+
## | GPU Name           | Util   Fan   Temp   Perf      Power       Memory |
## |=====+=====+=====+=====+=====+=====+=====+=====+=====|
## |    0 GeForce GTX 107... |  0%   39%   32C     P2     42W/252W   584/8116MiB |
## +-----+-----+-----+
##
## +-----+
## | GPU      PID  Type  Process name                               Mem Used |
## |=====+=====+=====+=====+=====+=====+=====+=====|
## |    0      1781    G  /usr/lib/xorg/Xorg                         273MiB |
## |    0     21407    C  /usr/lib/R/bin/exec/R                      311MiB |
## +-----+
```

cur

```
library(cur)

a = 1:10
b = integer(10)

x = cudaMalloc(10, "int")
cudaMemcpy(x, a, 10, "int", "hosttodevice")
cudaMemset(x, 0, 4, "int")
cudaMemcpy(b, x, 10, "int", "devicetohost")

b
## [1]  0  0  0  0  5  6  7  8  9 10
```

curand

```
n = 2.5e9
memuse:::howbig(n)
## 18.626 GiB

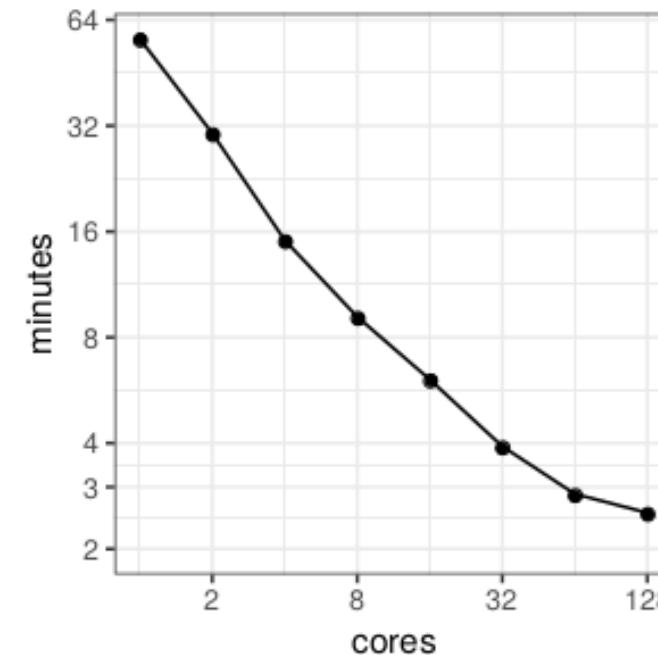
system.time(stats::rnorm(n))
## user  system elapsed
## 60.548   6.676  67.201

system.time(curand::runif(n))
## user  system elapsed
## 4.792   7.952 12.739
```

HOSVD* Workflow for a Fusion XGC1 Simulation Output

- Tensor dimensions:
 - 41 (time)
 - 32 (toroidal angle)
 - 232,011 (unstructured poloidal mesh)
 - Total size ~ 2.3 GB
- Workflow computations:
 - Read data from 41 HDF5 files
 - 5 SVD computations in series
 - 6 tensor unfoldings
 - 80 pdf plots (~3 MB each)
- Powered by R and pbdR packages
 - `pbdMPI`, `kazaam`, `launchr`

Strong scaling for complete workflow



- Not bad, considering no optimization
- Goal is to reach interactive speed

*

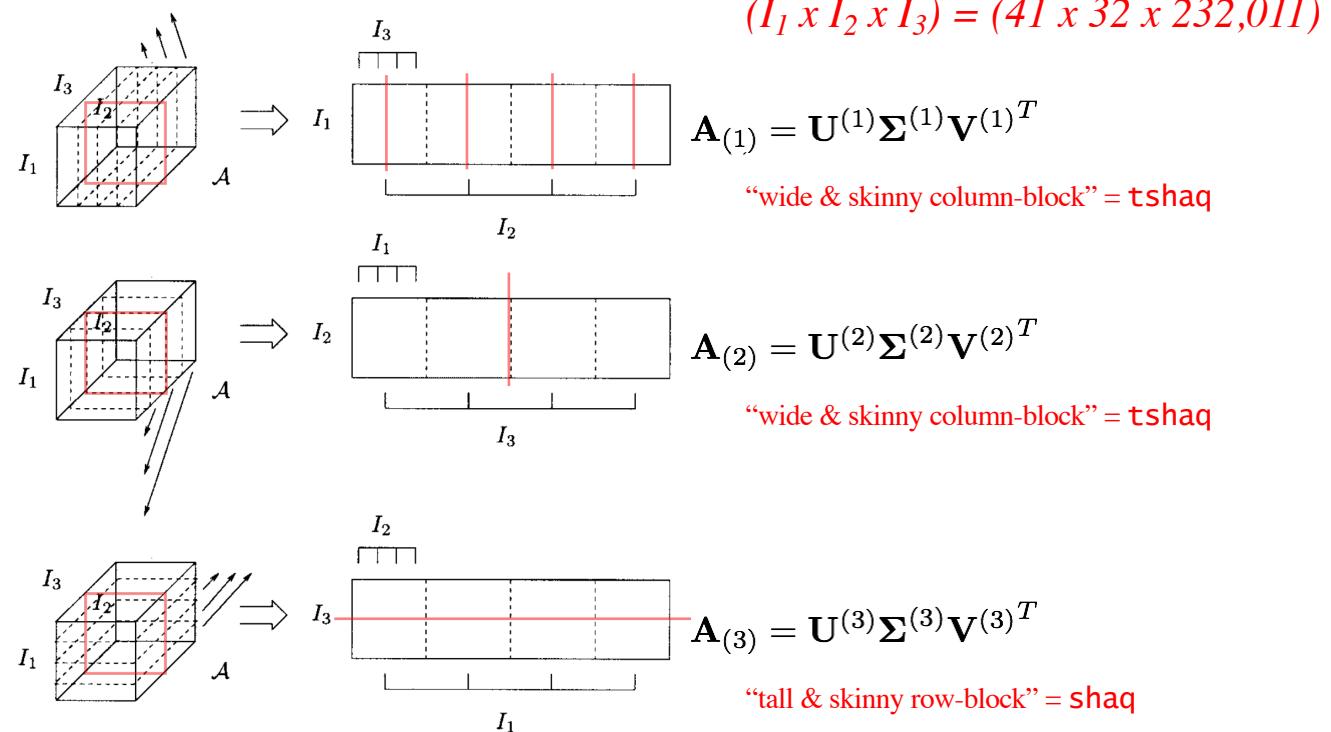
HOSVD: Higher Order Singular Value Decomposition

Higher Order SVD for a 3-D Array

$$\mathcal{A} = \mathcal{S} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{U}^{(3)}$$

FIG. 4. Visualization of the HOSVD for a third-order tensor.

Source: Lieven De Lathauwer, Bart De Moor, and Joos Vandewalle. A multilinear singular value decomposition. SIAM J. Matrix Anal. Appl., 21:1253-1278, 2000. (including figures)



Keep $\mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)}$ and compute $\mathcal{S} = \mathcal{A} \times_1 \mathbf{U}^{(1)T} \times_2 \mathbf{U}^{(2)T} \times_3 \mathbf{U}^{(3)T}$

Note that $(\mathcal{A} \times_i \mathbf{U}^{(i)})_{(i)} = \mathbf{U}^{(i)T} \mathbf{A}_{(i)}$

So that $\mathbf{S}_{(3)} = \mathbf{U}^{(3)T} (\mathbf{U}^{(2)T} (\mathbf{U}^{(1)T} \mathbf{A}_{(1)})_{(2)})_{(3)}$

Familiar Code but Cognizant of Distributed Dimension

$$\begin{aligned}\mathbf{A}_{(1)} &= \mathbf{U}^{(1)} \boldsymbol{\Sigma}^{(1)} \mathbf{V}^{(1)T} \\ \mathbf{A}_{(2)} &= \mathbf{U}^{(2)} \boldsymbol{\Sigma}^{(2)} \mathbf{V}^{(2)T} \\ \mathbf{A}_{(3)} &= \mathbf{U}^{(3)} \boldsymbol{\Sigma}^{(3)} \mathbf{V}^{(3)T}\end{aligned}$$

Keep $\mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)}$ and compute the \mathcal{S}

$$\mathcal{S} = \mathcal{A} \times_1 \mathbf{U}^{(1)T} \times_2 \mathbf{U}^{(2)T} \times_3 \mathbf{U}^{(3)T}$$

Note that $(\mathcal{A} \times_i \mathbf{U}^{(i)})_{(i)} = \mathbf{U}^{(i)T} \mathbf{A}_{(i)}$
So $\mathbf{S}_{(3)} = \mathbf{U}^{(3)T} (\mathbf{U}^{(2)T} (\mathbf{U}^{(1)T} \mathbf{A}_{(1)})_{(2)})_{(3)}$

```
library(kazaam)
tens = read_xgc_window(file_var, var, w_center, window)$Data
tdim = dim(tens) # local dimensions (1, 2, 3d)

## A1 unfolding and SVD
A1 = as.vector(tens) # (1*2*3d)
dim(A1) = c(tdim[1], tdim[2]*tdim[3]) # (1, 2*3d)
U1 = svd(tshaq(A1))$u # (1, 2*3d) tshaq => (1, 1)

re_ord = . . . # index for 1*2 => 2*1
re_ord_inv = . . . # index for 2*1 => 1*2
## A2 unfolding and SVD
. . .
U2 = . . .
## A3 unfolding and SVD
. . .
U3 = . . .

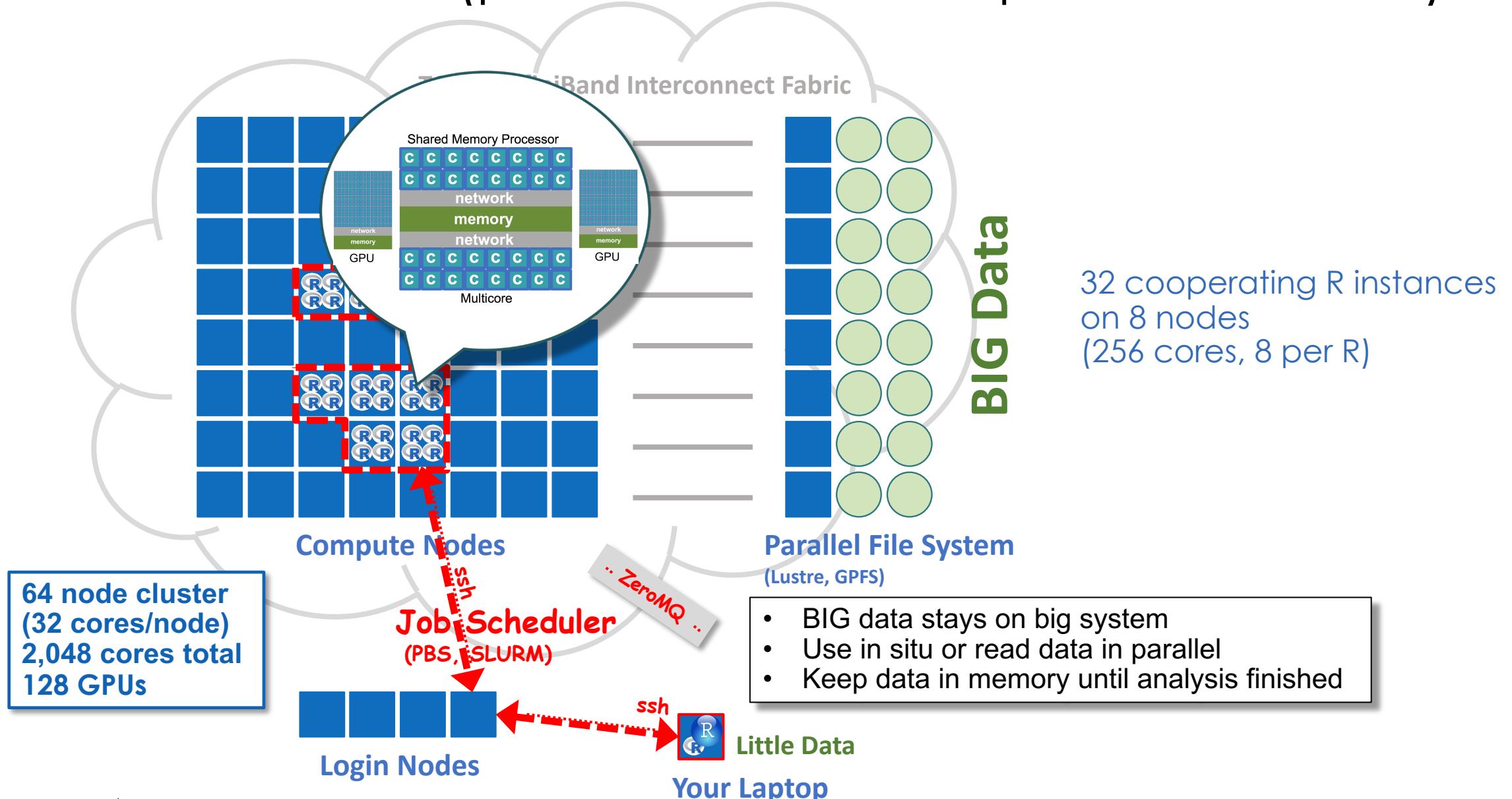
## Core tensor computation
S1 = crossprod(U1, A1) # t((1, 1)) %*% (1, 2*3d)
S1 = as.vector(S1) # (1*2*3d)
dim(S1) = c(tdim[1]*tdim[2], tdim[3]) # (1*2, 3d)

S2 = S1[re_ord, ] # (1*2, 3d) => (2*1, 3d)
dim(S2) = c(tdim[2], tdim[1]*tdim[3]) # (2, 1*3d)
S2 = crossprod(U2, S2) # t((2, 2)) %*% (2, 1*3d)

S3 = as.vector(S2) # (2, 1, 3d)
dim(S3) = c(tdim[2]*tdim[1], tdim[3]) # (2*1, 3d)
S3 = S3[re_ord_inv, ] # (2*1, 3d) => (1*2, 3d)
S3 = crossprod(U3, shaq(t(S3))) # t((3d, 3c)) %*% t((1*2, 3d)) shaq = (3c, 1*2)

S = t(S3) # dim (3c, 1*2) => (1*2, 3c)
dim(S) = c(tdim[1], tdim[2], min(tdim[1]*tdim[2], allreduce(tdim[3])))
```

Interactive SPMD (pbdZMQ, remoter, pbdCS, launchr)



pbdR Project Support



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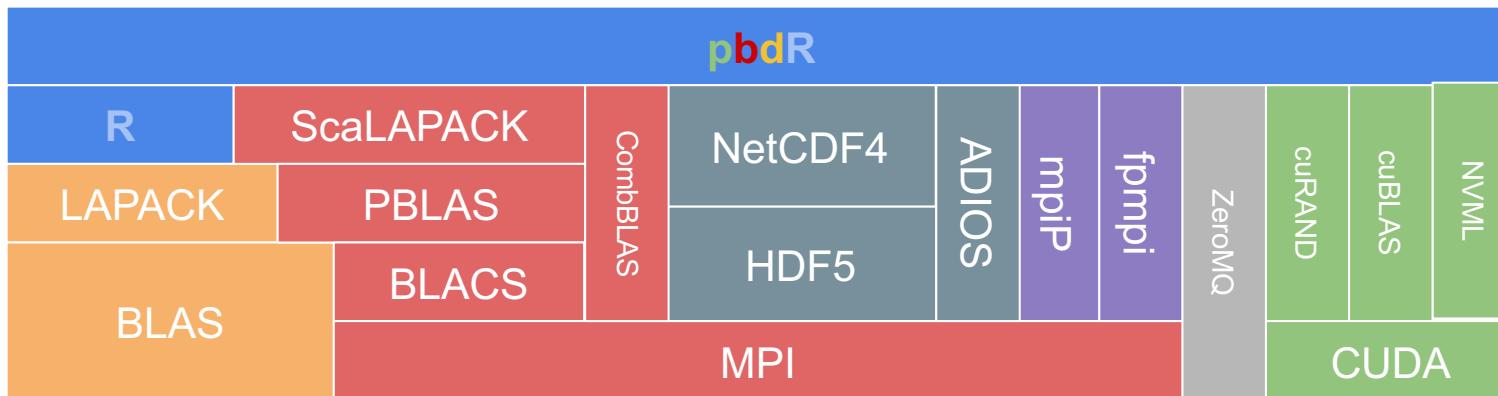
Resources:

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Thank You!



Distinctions

- A component of 2019 Cray® Urika®-CS AI and Analytics Suite
- Intel® HPC Developer Conference 2017: People's Choice Award, High Productivity Languages Track
- 2016 ORNL Significant Event Award
- Benchmark code for Frontier procurement

ORNL Installations

- Supported software on OLCF platforms (Rhea, Eos, Titan, Summit)
- Available on CADES resources
- Install from: <https://pbdR.org/releases>



Schmidt, Chen, Matheson, and Ostroumov (2017). Programming with BIG Data in R: Scaling Analytics from One to Thousands of Nodes. *Big Data Research*, vol.8, p.1-11.

Schmidt, Chen, and Ostroumov (2016). Introducing a New Client/Server Framework for Big Data Analytics with the R Language. *XSEDE16 Conference on Diversity, Big Data, and Science at Scale*, Article No. 38.