Elevating R to Supercomputers

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The pbdR Core Team

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Programming with Big Data in R

Support

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Contents

1 Introduction

2 Benchmarks

3 Challenges

Why R?

Why R?

1. Because.

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2. R community has growing data size problem.

Why R?

1. Because.
2. R community has growing data size problem.
3. HPC community has growing need for data analytics.

Elevating R to Supercomputers

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1. Existing code.

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2. Syntax.

Elevating R to Supercomputers

1. Existing code.
2. Syntax.
3. Philosophy.

Programming with Big Data in R (pbdR)

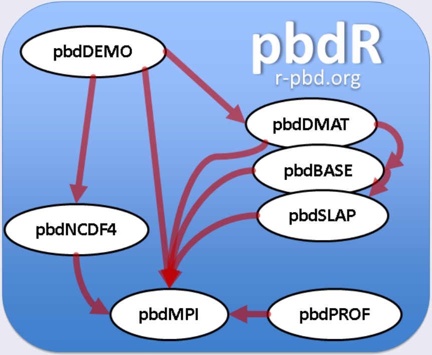
Productivity, Portability, Performance

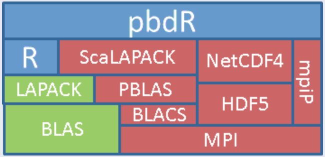
pbdR
Programming with Big Data in R

- *Free*[a] R packages.
- Bridging high-performance C with high-productivity of R
- Distributed data details implicitly managed.
- Methods have syntax *identical* to R.

[a] MPL, BSD, and GPL licensed

pbdR Packages





pbdMPI vs Rmpi: API

pbdMPI vs Rmpi: API

Reduction Operations

Rmpi

```
# int
mpi.allreduce(x, type=1)
# double
mpi.allreduce(x, type=2)
```

pbdMPI

```
allreduce(x)
```

pbdMPI vs Rmpi: API

Reduction Operations

Rmpi

```
# int
mpi.allreduce(x, type=1)
# double
mpi.allreduce(x, type=2)
```

pbdMPI

```
allreduce(x)
```

Types in R

```
> is.integer(1)
[1] FALSE
> is.integer(2)
[1] FALSE
> is.integer(1:2)
[1] TRUE
```

pbdMPI vs Rmpi: Performance

Table: Runtimes (seconds) for $10,000 \times 10,000$ `allgather` with **Rmpi** and **pbdMPI**.

Cores	**Rmpi**	**pbdMPI**	Speedup
32	24.6	6.7	3.67
64	25.2	7.1	3.55
128	22.3	7.2	3.10
256	22.4	7.1	3.15

pbdR Example Syntax

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

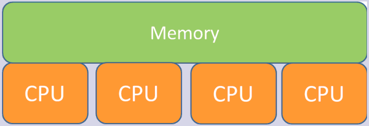
Look familiar?

The above runs on 1 core with R or 10,000 cores with pbdR

Shared and Distributed Memory Machines

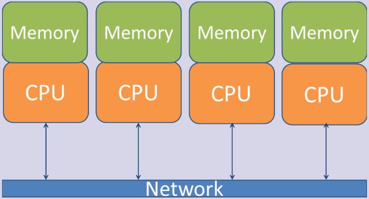
Shared Memory

Direct access to read/change memory (one node)



Distributed

No direct access to read/change memory.



Shared and Distributed Memory Machines

Shared Memory Machines

Thousands of cores

Nautilus, University of Tennessee
1024 cores
4 TB RAM

Distributed Memory Machines

Hundreds of thousands of cores

Kraken, University of Tennessee
112,896 cores
147 TB RAM

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Non-Optimal Choices Throughout

1. Only libre software used (no MKL, ACML, etc.).

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1. Only libre software used (no MKL, ACML, etc.).
2. 1 core = 1 MPI process.
3. No tuning for data distribution.

Benchmark Data

1. Random normal $N(100, 10000)$.

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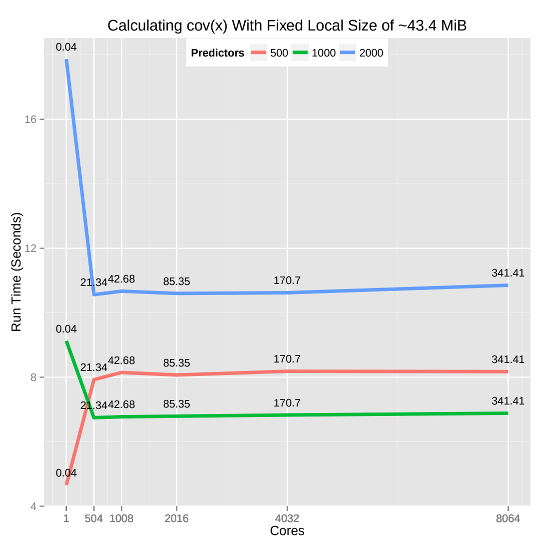
1. Random normal $N(100, 10000)$.
2. Local problem size of $\approx 43.4MiB$.
3. Three sets: 500, 1000, and 2000 columns.
4. Several runs at different core sizes within each set.

Covariance Code

```r
x <- ddmatrix("rnorm", nrow=n, ncol=p, mean=mean, sd=sd)

cov.x <- cov(x)
```

cov()


Calculating cov(x) With Fixed Local Size of ~43.4 MiB
Predictors
500
1000
2000
Run Time (Seconds)
Cores
16
12
8
4
1
504
1008
2016
4032
8064
0.04
21.34
42.68
85.35
170.7
341.41
0.04
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21.34
42.68
85.35
170.7
341.41
0.04

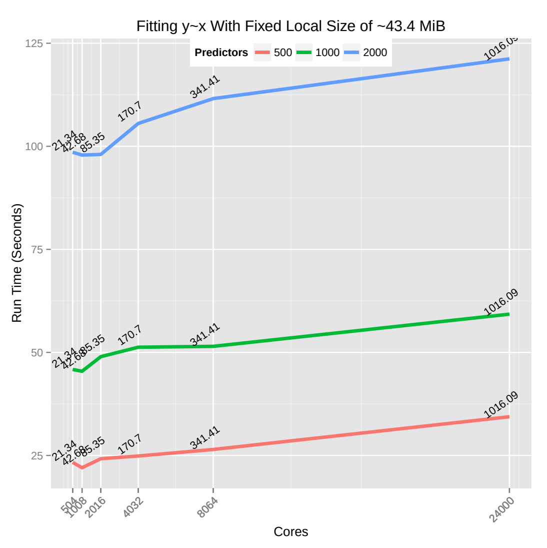
Linear Model Code

```r
x <- ddmatrix("rnorm", nrow=n, ncol=p, mean=mean, sd=sd)
beta_true <- ddmatrix("runif", nrow=p, ncol=1)

y <- x %*% beta_true

beta_est <- lm.fit(x=x, y=y)$coefficients
```

lm.fit()


Fitting y~x With Fixed Local Size of ~43.4 MiB
Predictors 500 1000 2000
Run Time (Seconds)
125
100
75
50
25
Cores
504
1008
2016
4032
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170.7
341.41
1016.09

But wait! There's more...

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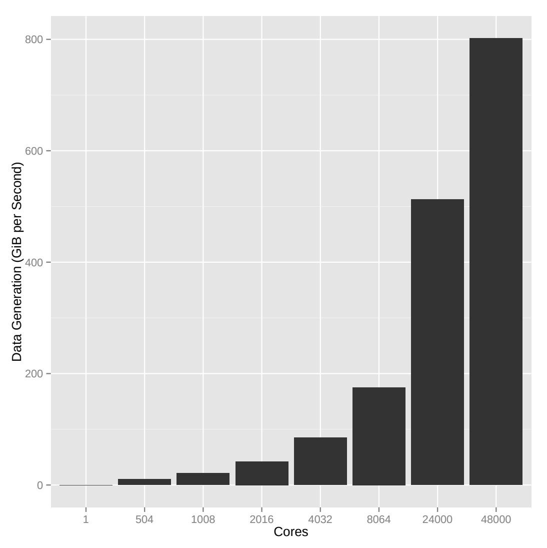
Anything worth doing is worth overdoing.

— Mick Jagger

Data Generation



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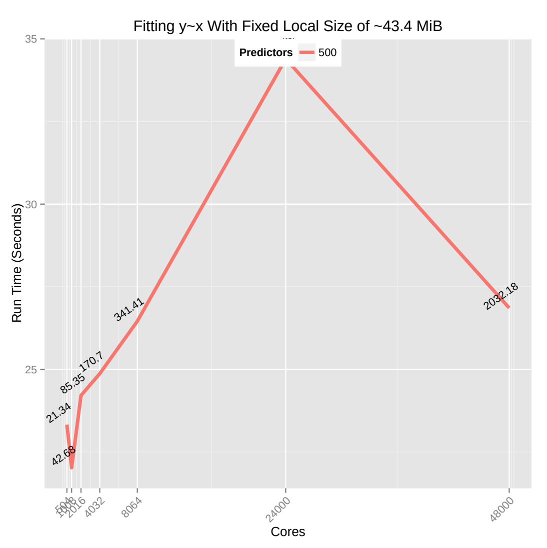
Fitting y~x With Fixed Local Size of ~43.4 MiB
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2016
4032
8064
24000
48000
Cores

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- Perceptions.
  "*R? Isn't that slow?*" – HPC people
  "*HPC? Isn't that hard?*" – R people

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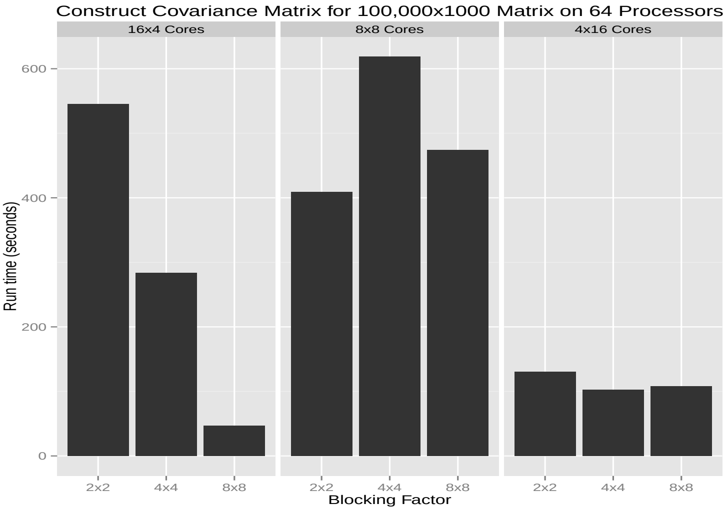
- Perceptions.
  "*R? Isn't that slow?*" – HPC people
  "*HPC? Isn't that hard?*" – R people
- Package loading.
- Profiling.
- Data distribution and performance.

Covariance Revisited: Distributed Data Parameter Calibration



Thanks for coming!

Questions?

http://r-pbd.org/