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

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

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

Programming with Big Data in R (pbdR)

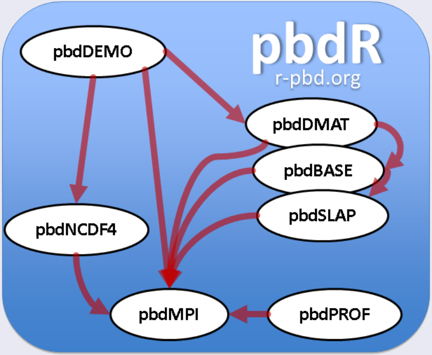
Productivity, Portability, Performance

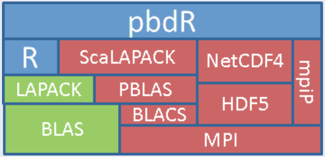
Programming with Big Data in R

- *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

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

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

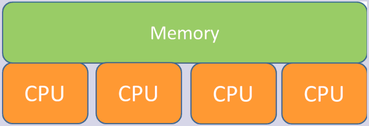
Look familiar?

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

Shared and Distributed Memory Machines

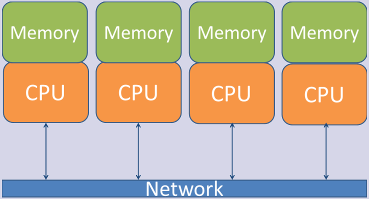
Shared Memory

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

Contents

Non-Optimal Choices Throughout

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

Benchmark Data

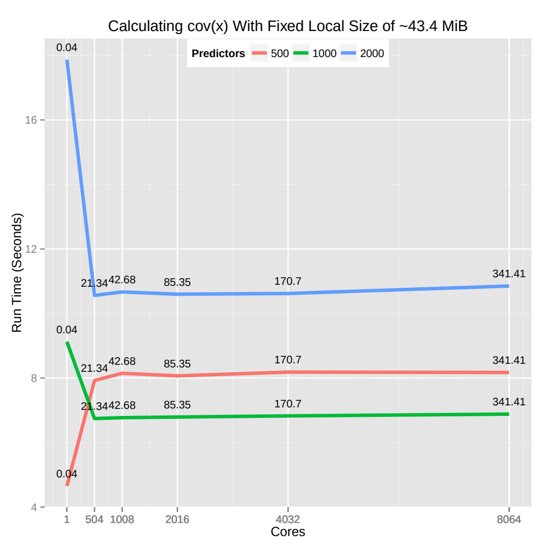
1. Random normal $N(100, 10000)$.
2. Local problem size of $\approx 43.4 MiB$.
3. Three sets: 500, 1000, and 2000 columns.
4. Several runs at different core sizes within each set.

Covariance Code

```
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)
16
12
8
4
0.04
21.34
42.68
85.35
170.7
341.41
1 504 1008 2016 4032 8064
Cores

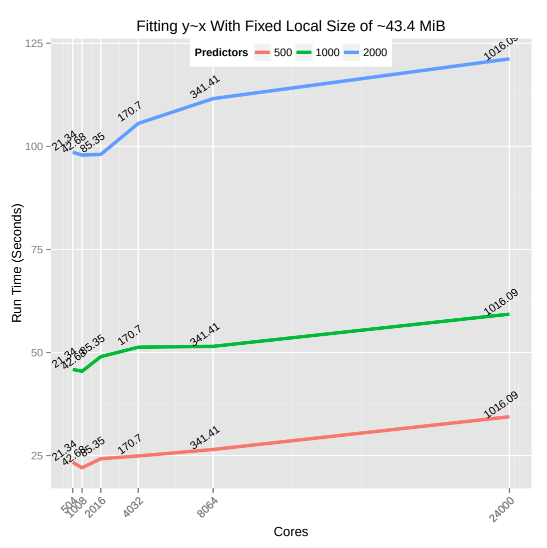
Linear Model Code

```
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()

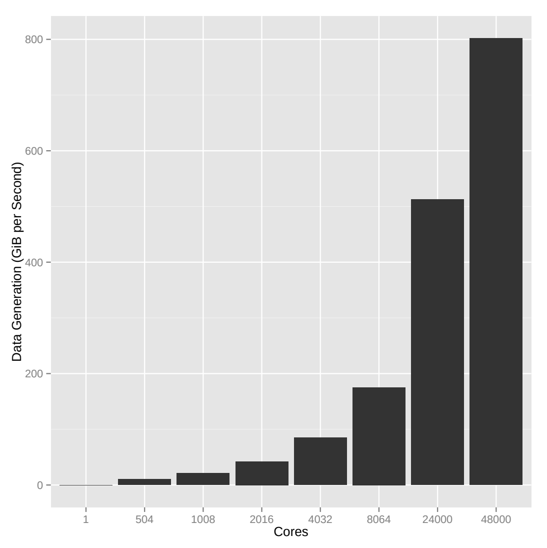

Fitting y~x With Fixed Local Size of ~43.4 MiB
Predictors 500 1000 2000
Run Time (Seconds)
125
100
75
50
25
Cores
504
1008
2016
4032
8064
24000
21.34
42.68
85.35
170.7
341.41
1016.09

But wait! There's more...

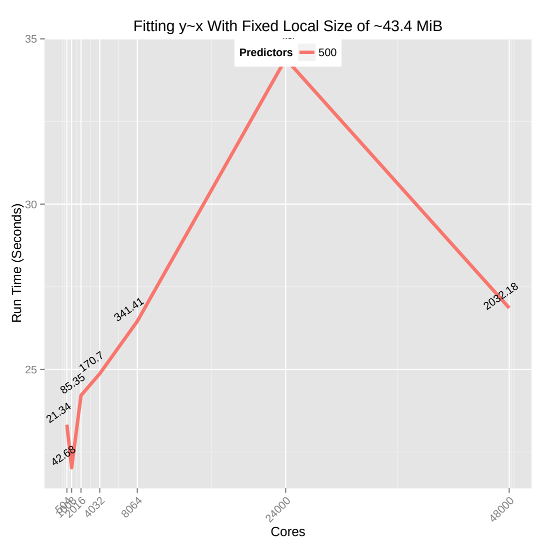
Anything worth doing is worth overdoing.

— Mick Jagger

Data Generation



lm.fit()

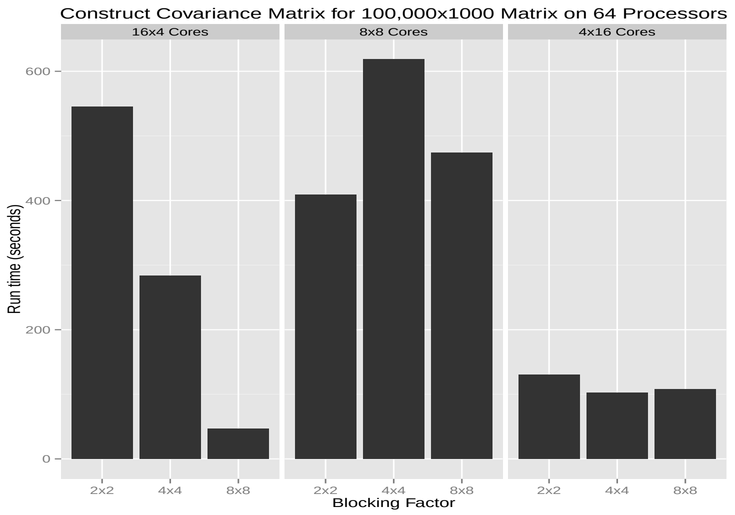

Fitting y~x With Fixed Local Size of ~43.4 MiB
Predictors
500
Run Time (Seconds)
35
30
25
21.34
42.68
85.35
170.7
341.41
2032.18
504
1008
2016
4032
8064
24000
48000
Cores

Contents

Challenges

- 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/