From 1 Core to Thousands: R to pbdR

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Affiliations and Support

The pbdR Core Team
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About This Presentation

Downloads

This presentation and supplemental materials are available at:

http://r-pbd.org/tutorial

Sample R scripts and pbs job scripts available on Nautilus from:

/lustre/medusa/mschmid3/tutorial/scripts.tar.gz

Contents

Contents

What is R?

- *lingua franca* for data analytics and statistical computing.
- Part programming language, part data analysis package.
- Dialect of S (Bell Labs).
- Syntax designed for data. scoping semantics, and 2 official OOP systems.

Who uses R?

Google, Pfizer, Merck, Bank of America, Shell[a],
Oracle[b], Facebook, bing, Mozilla, okcupid[c] ,
ebay[d],
kickstarter[e], the New York Times[f]

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[a] https://www.nytimes.com/2009/01/07/technology/business-computing/07program.html?_r=0

[b] http://www.oracle.com/us/corporate/features/features-oracle-r-enterprise-498732.html

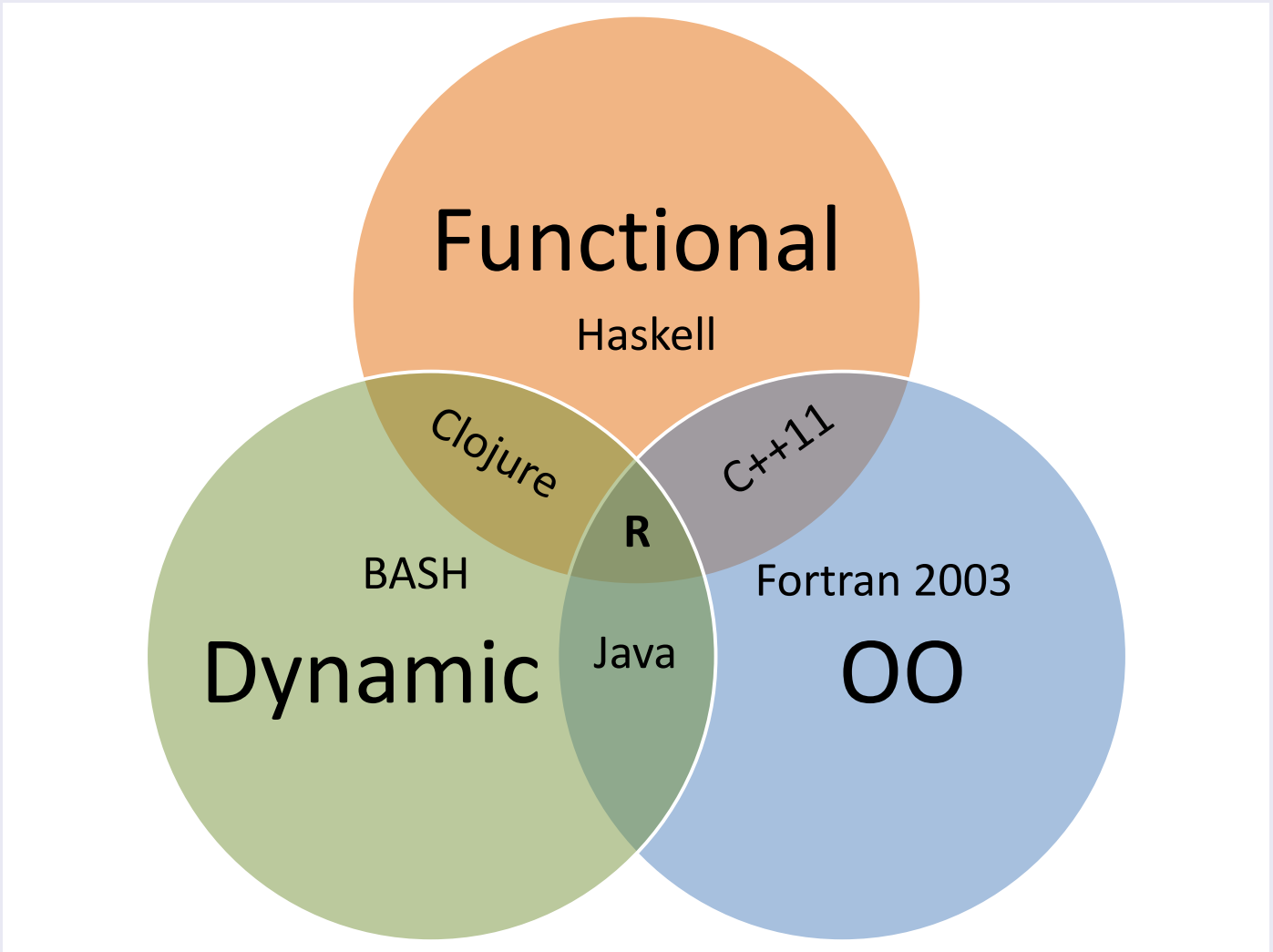
[c] http://www.revolutionanalytics.com/what-is-open-source-r/companies-using-r.php

[d] http://blog.revolutionanalytics.com/2012/09/using-r-in-production-industry-experts-share-their-experiences.html

[e] http://blog.revolutionanalytics.com/2012/09/kickstarter-facilitates-50m-in-indie-game-funding.html

[f] http://blog.revolutionanalytics.com/2012/05/nyt-charts-the-facebook-ipo-with-r.html

Language Paradigms



Data Types

- Storage: logical, int, double, double complex, character
- Structures: vector, matrix, array, list, dataframe
- Caveats: (Logical) `TRUE`, `FALSE`, `NA`

For the remainder of the tutorial, we will restrict ourselves to real number matrix computations.

High Level Syntax

```
1 x <- matrix(rnorm(30), nrow=10)
2 x <- x[-1, 2:5]
3 x <- log(abs(x) + 1)
4 xtx <- t(x) %*% x
5 ans <- svd(solve(xtx))
```

More than just a Matlab clone...

- Data science (machine learning, statistics, data mining, ...) is mostly matrix algebra.

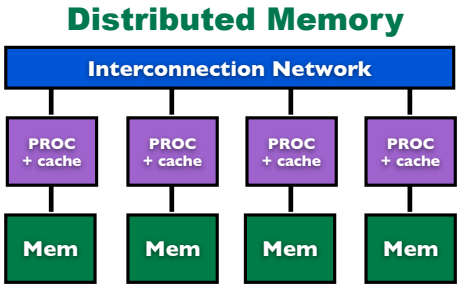
  So what about Matlab/Python/Julia/...?
- Depends on your "religion"
- As a *data analysis* package, R is king.

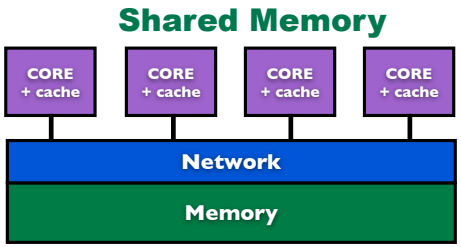
High Level Syntax *for Data*

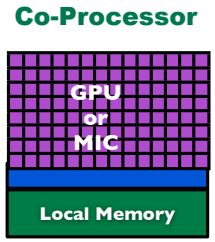
```
1 pca <- prcomp(x, retx=TRUE, scale=TRUE)
2 prop_var <- cumsum(pca$sdev)/sum(pca$sdev)
3 i <- min(which(prop_var > 0.9)) - 1
4
5 y <- pca$x[, 1:i]
```

Contents

Three Basic Flavors of Hardware



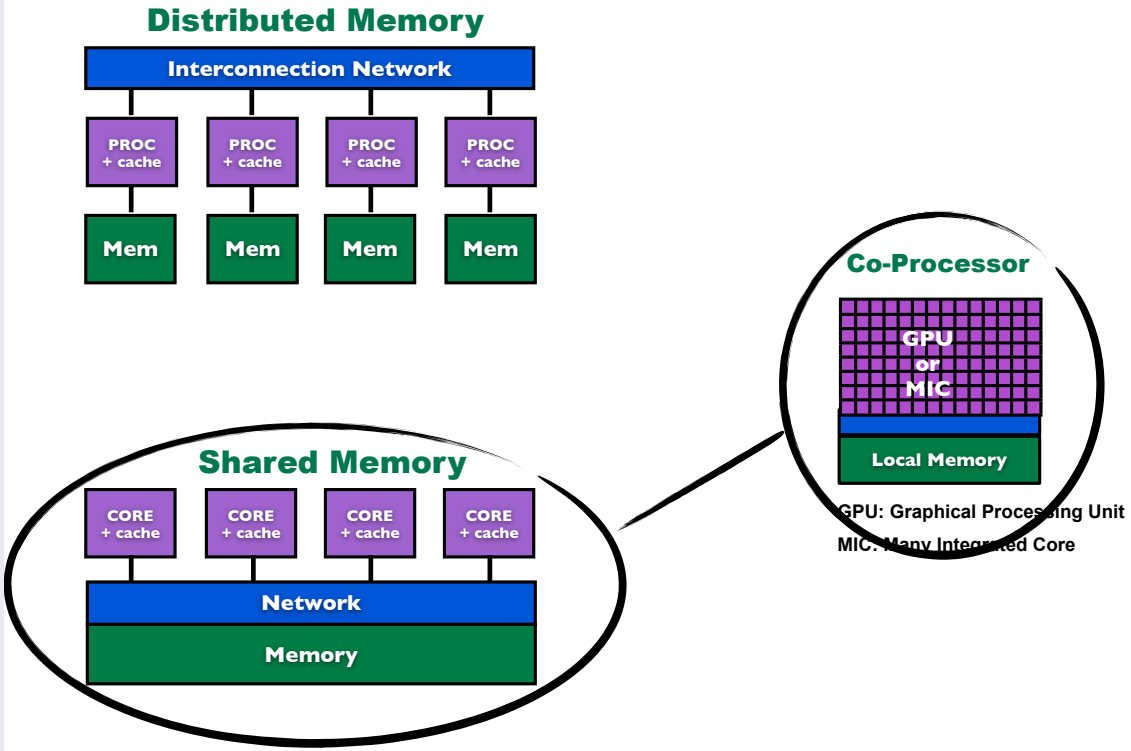




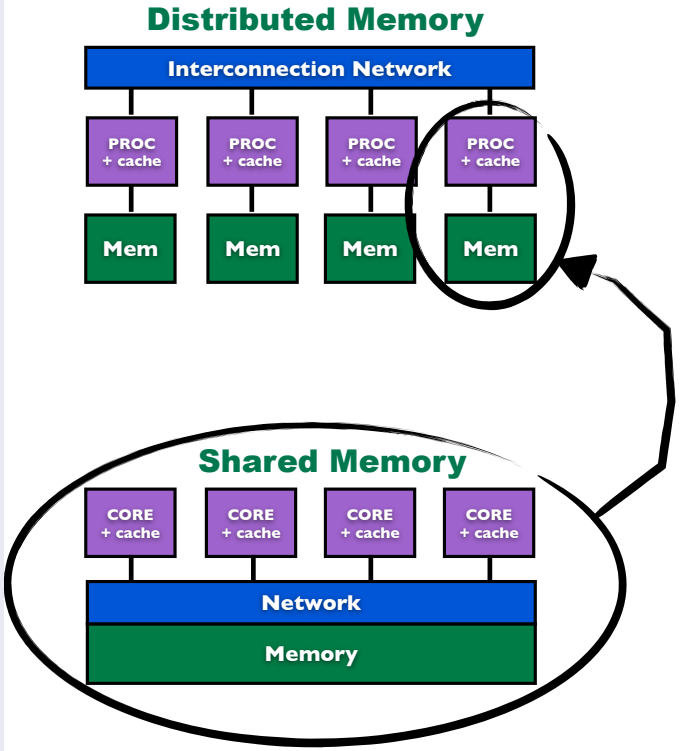
GPU: Graphical Processing Unit

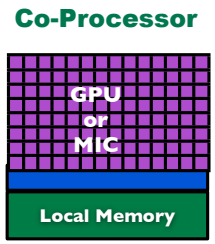
MIC: Many Integrated Core

Your Laptop or Desktop



A Server or Cluster

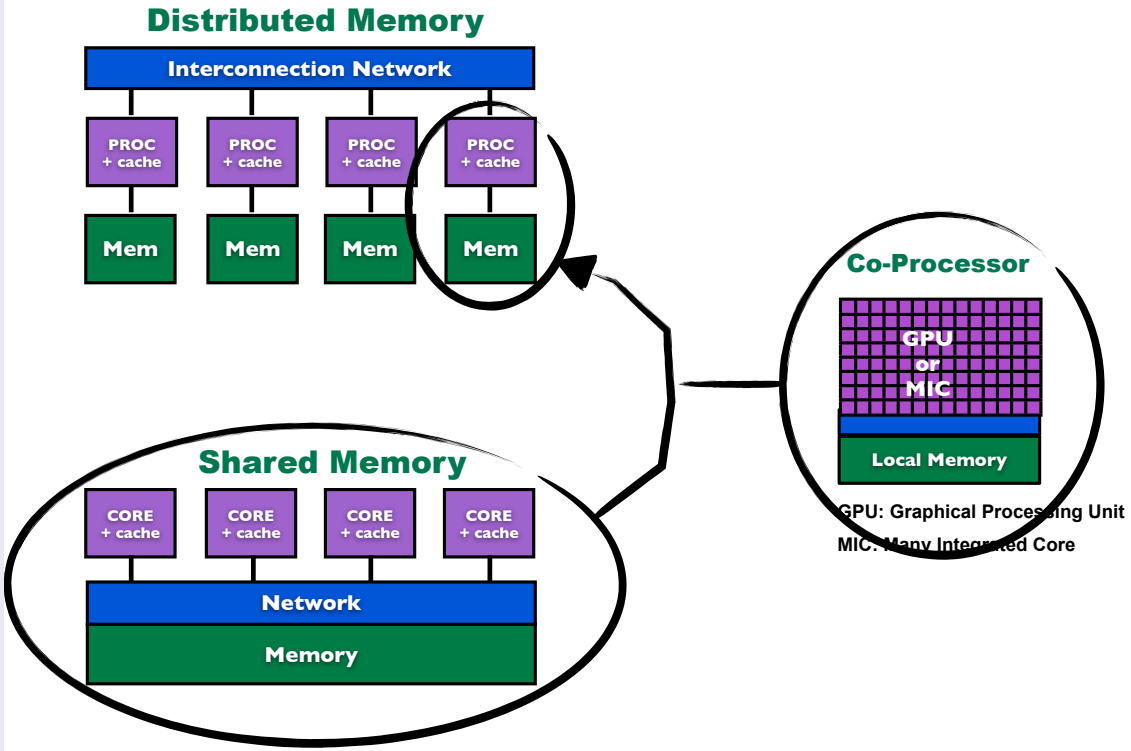




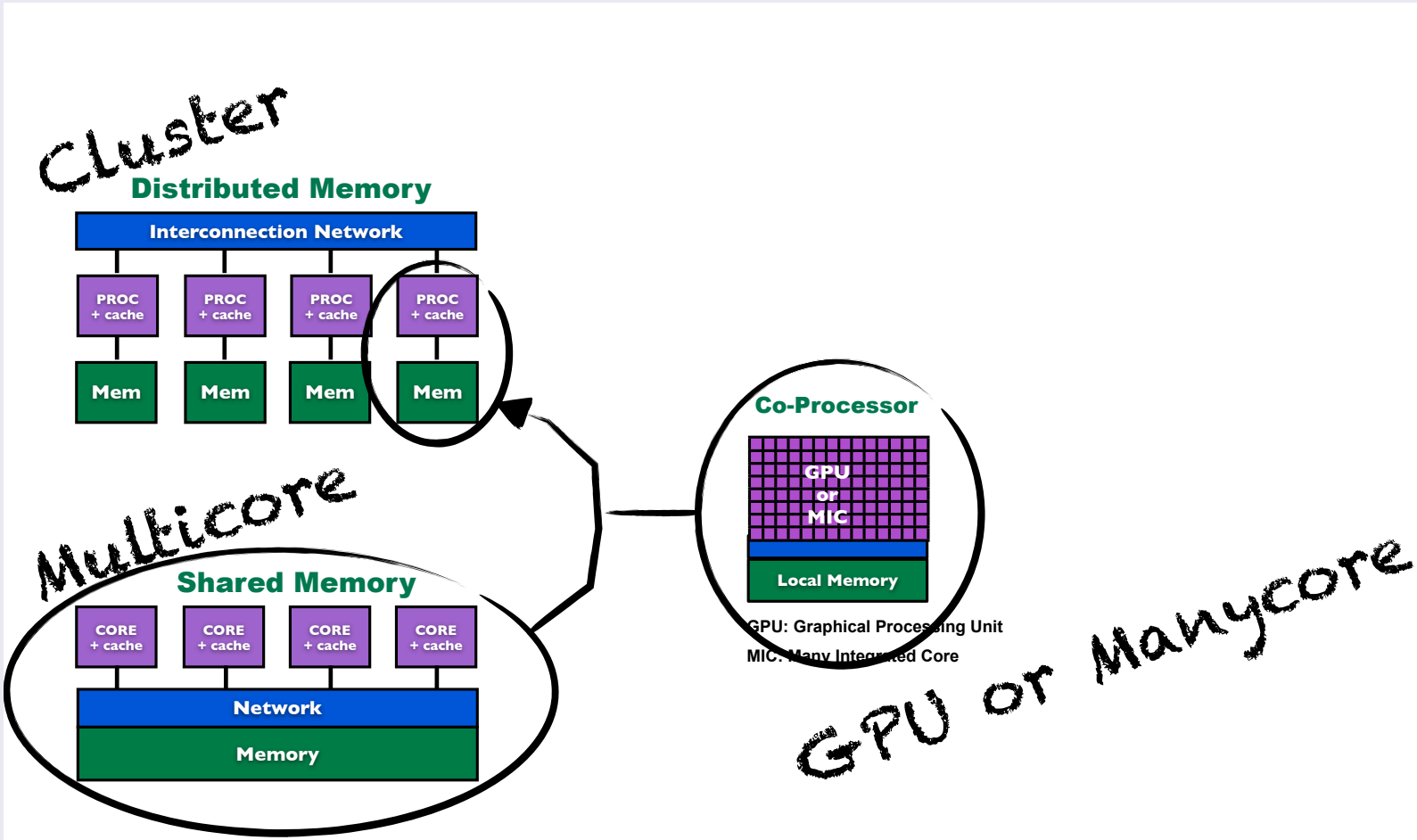
GPU: Graphical Processing Unit

MIC: Many Integrated Core

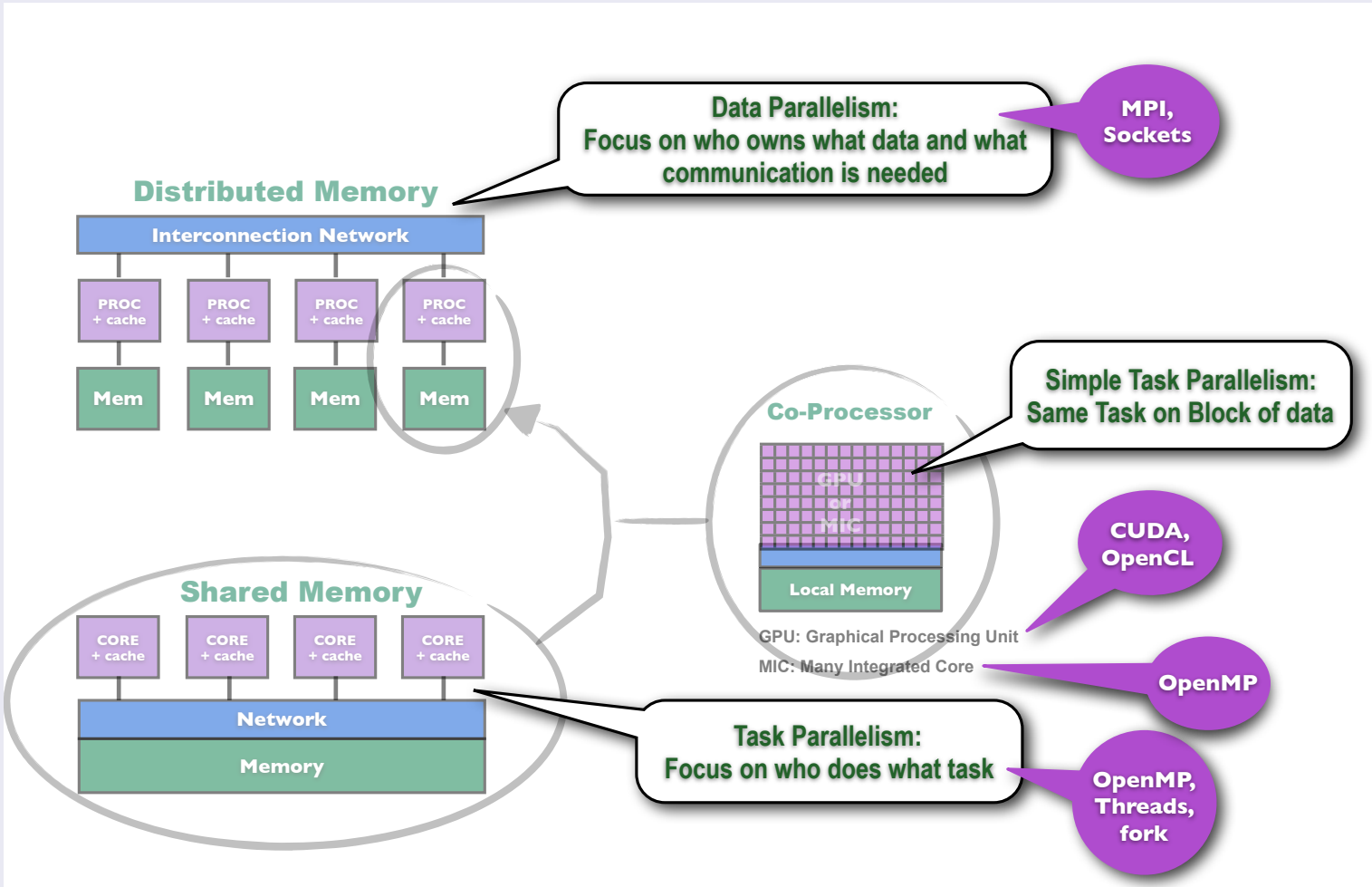
Server to Supercomputer



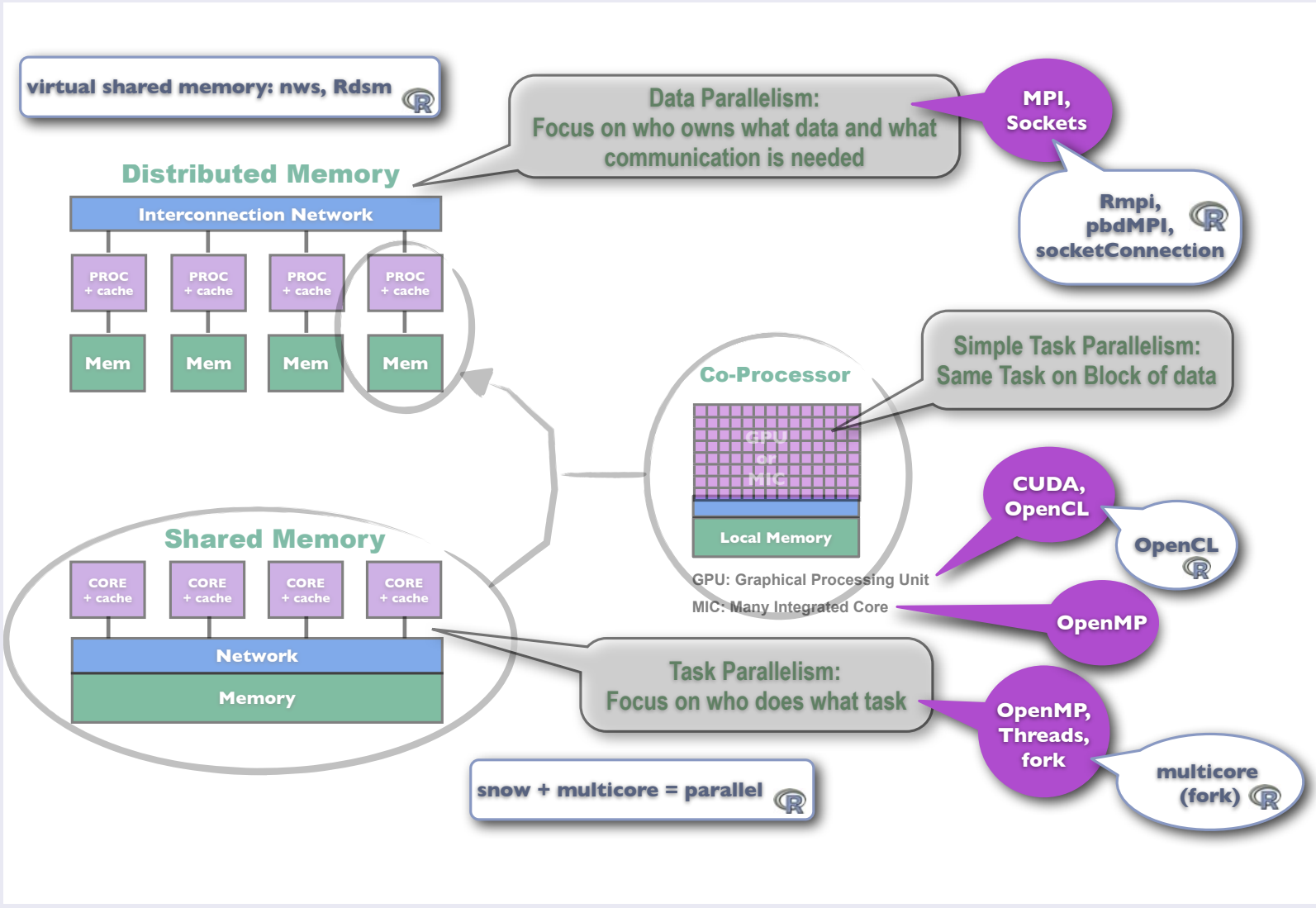
Knowing the Right Words



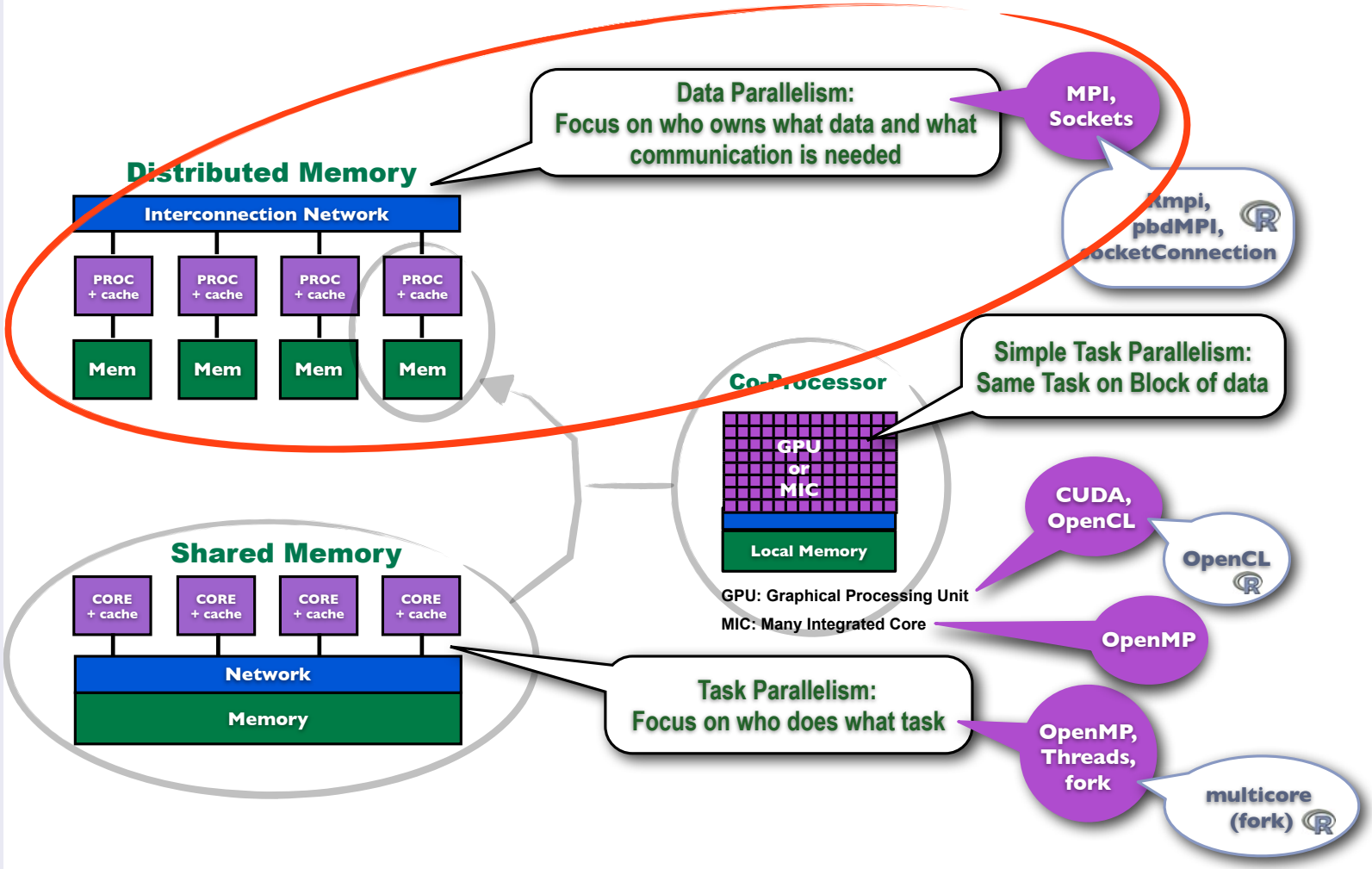
"Native" Programming Models and Tools



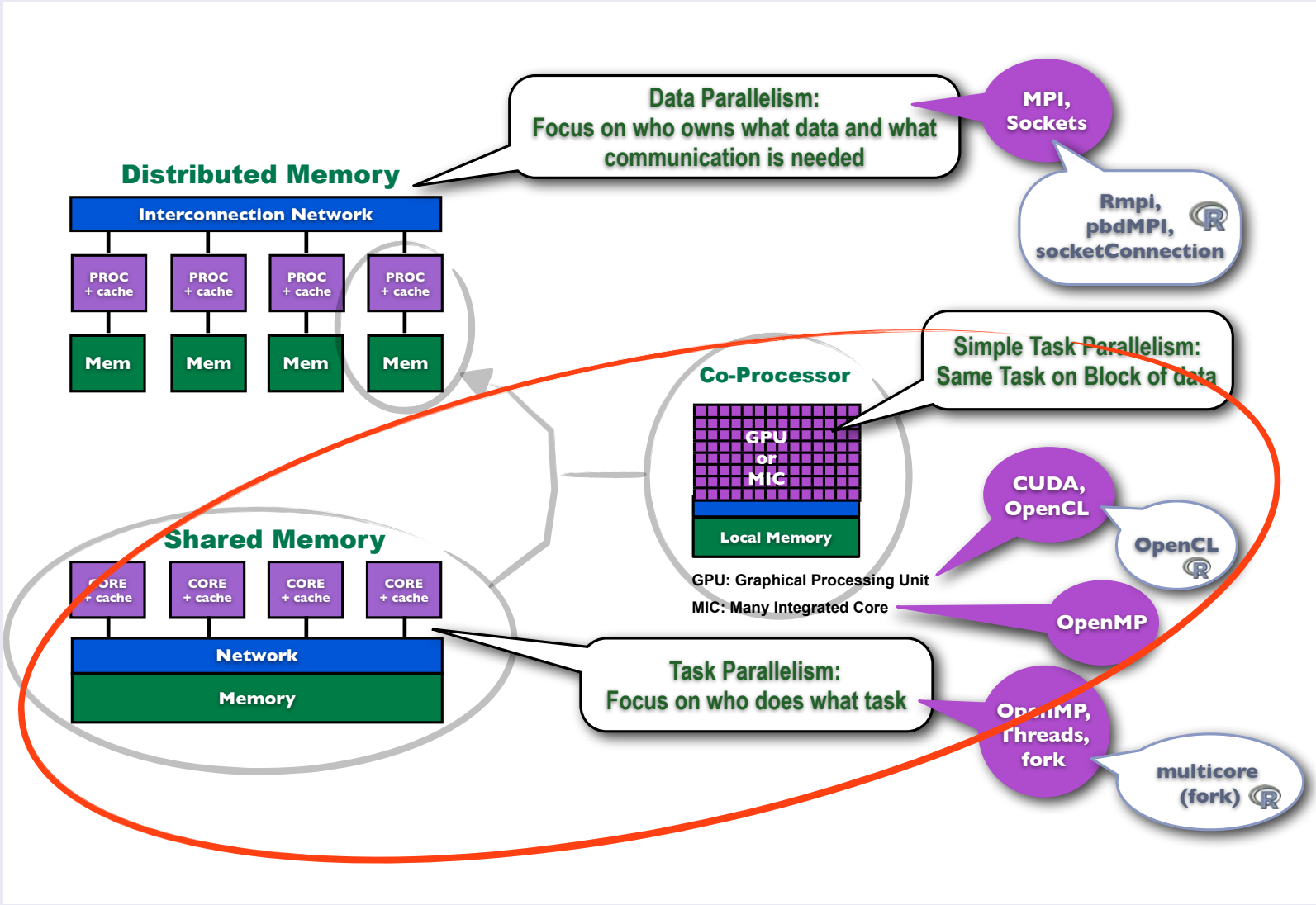
R Interfaces to Native Tools



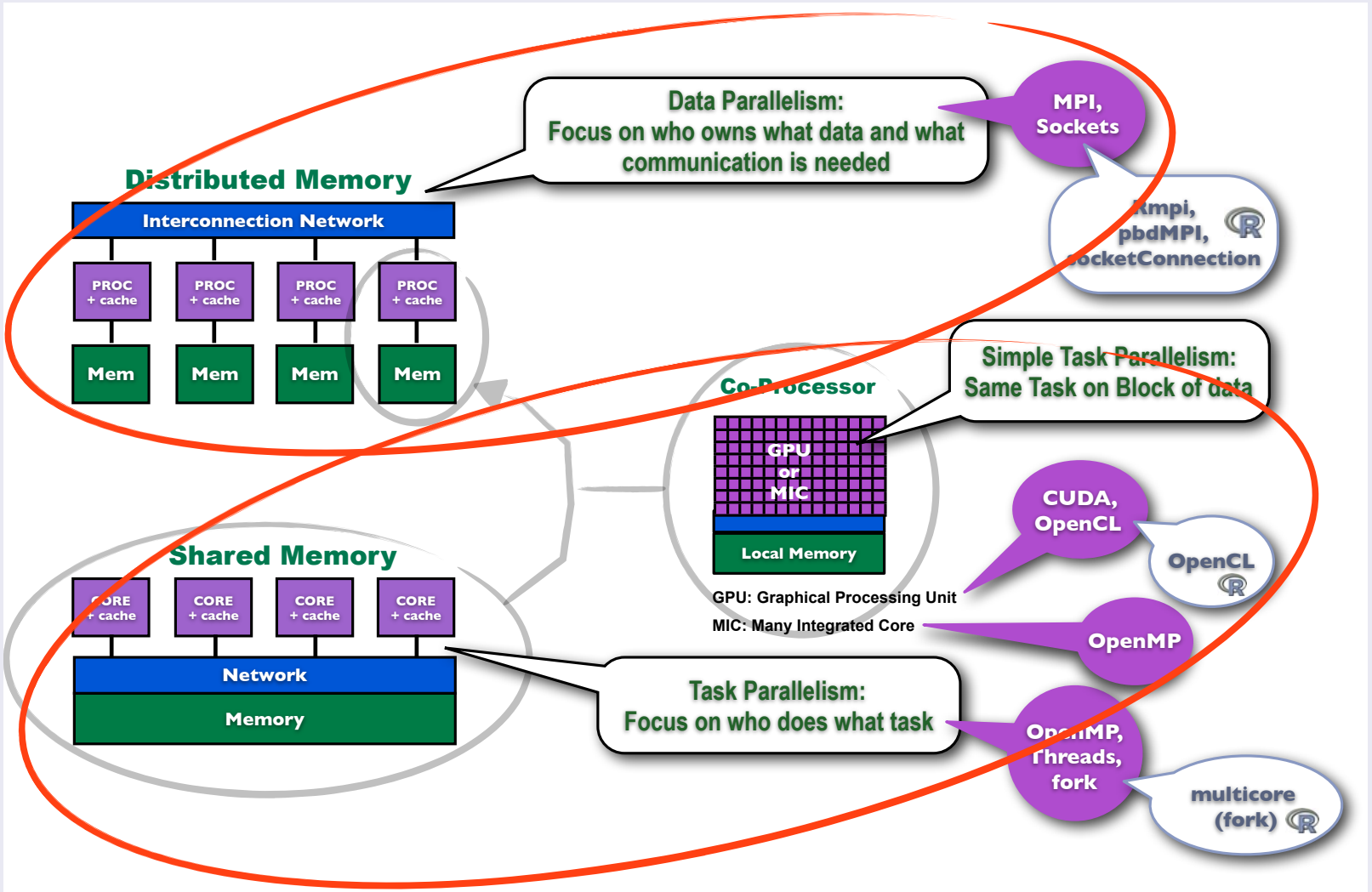
30+ Years of Parallel Computing Research



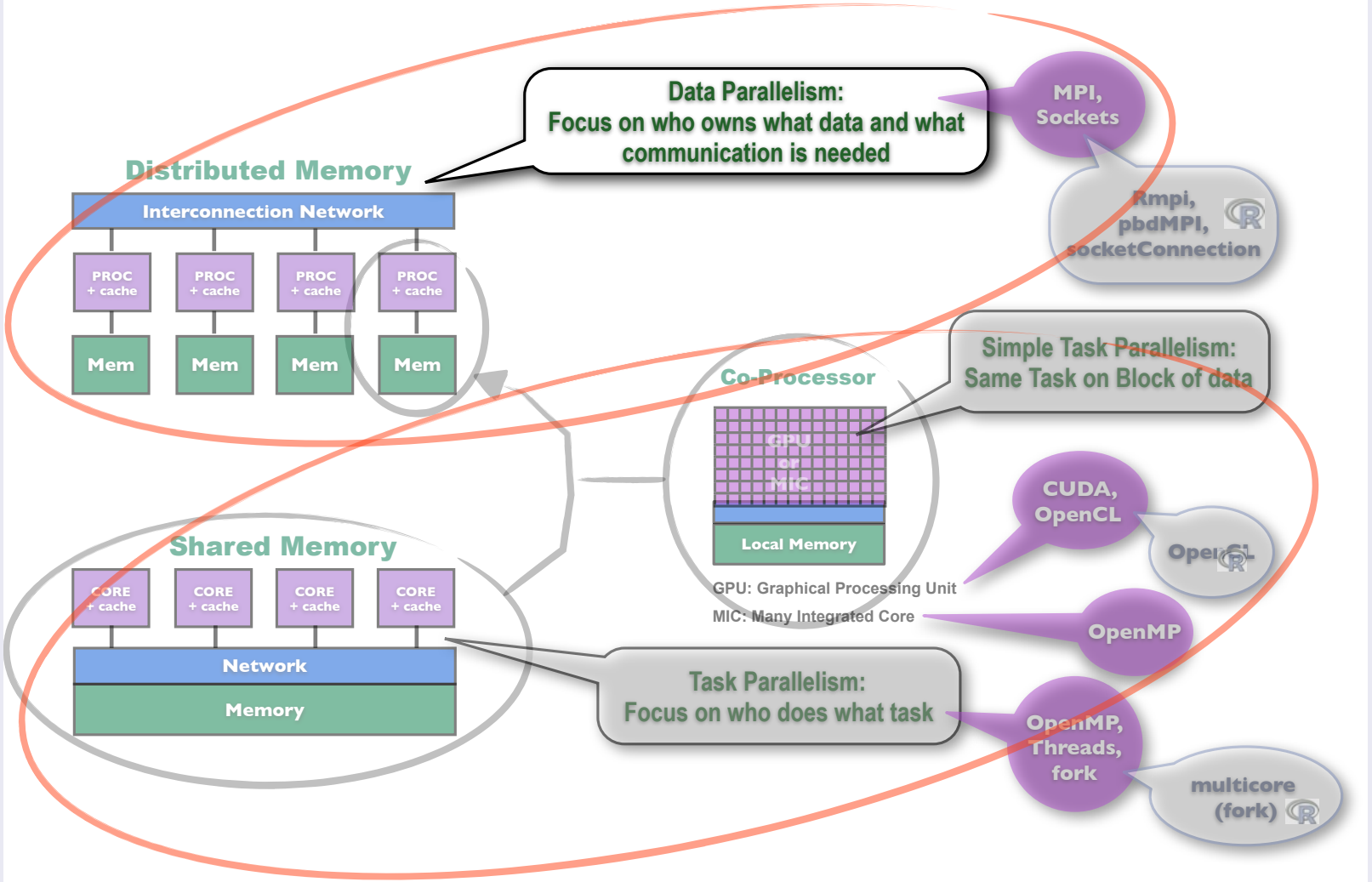
Last 10 years of Advances



Putting It All Together Challenge



pbdR Focus on Data Parallelism



Contents

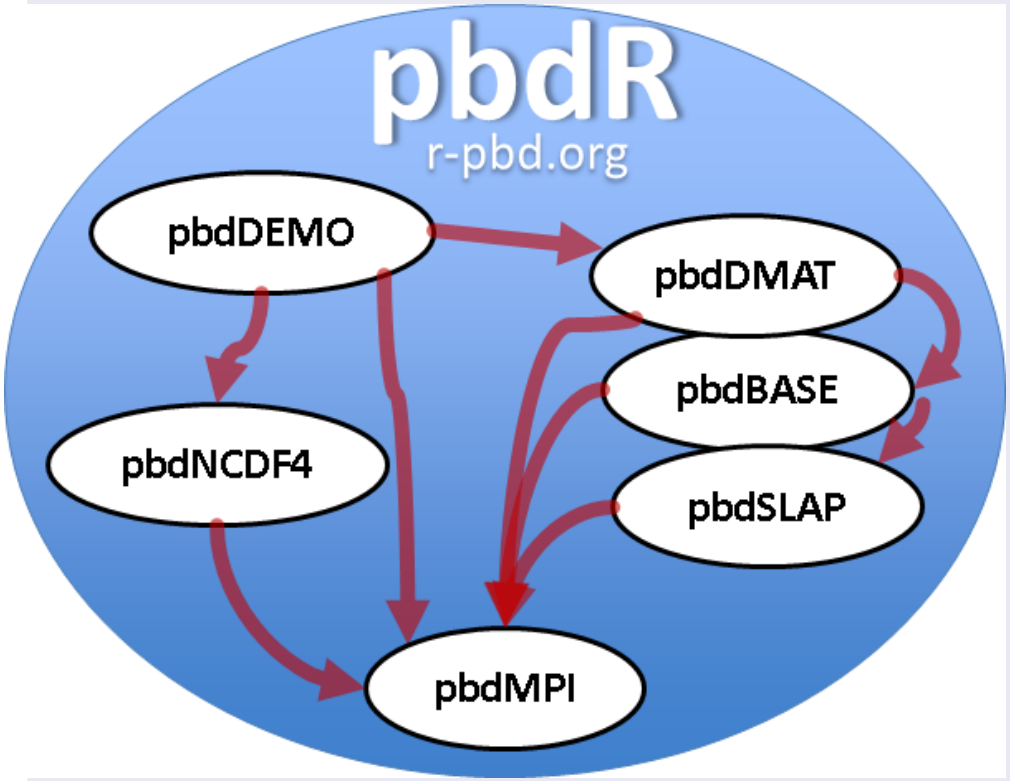
Programming with Big Data in R (pbdR)

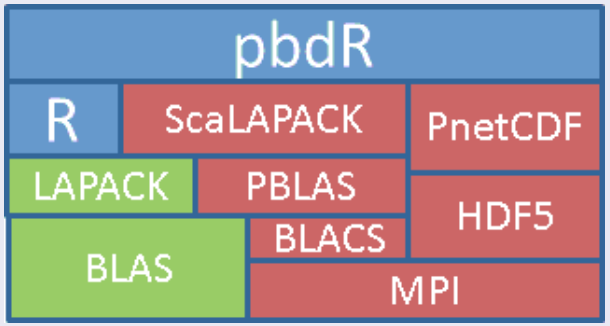
Striving for *Productivity, Portability, Performance*

- *Free*[a] R packages.
- Bridging high-performance C with high-productivity of R
- Scalable, big data analytics.
- Distributed data details implicitly managed.
- Methods have syntax *identical* to R.
- Powered by state of the art numerical libraries (MPI, ScaLAPACK, . . .)

[a] MPL, BSD, and GPL licensed

pbdR Packages





pbdR on HPC Resources

pbdR is currently installed and maintained on:

- Nautilus, UTK
- Kraken, UTK
- Newton, UTK
- Lens, ORNL
- Titan, ORNL
- tara, UMBC

If you are interested in maintaining pbdR, contact us at RBigData@gmail.com

Example Syntax

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

Look familiar?

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

pbdR Paradigms

Programs that use pbdR utilize:

- Batch execution
- Single Program/Multiple Data (SPMD) style

And generally utilize:

- Data Parallelism

Batch Execution

- Non-interactive
- Use

```
Rscript my_script.r
```

or

```
R CMD BATCH my_script.r
```

- In parallel:

```
mpirun -np 2 Rscript my_par_script.r
```

Single Program/Multiple Data (SPMD)

- Difficult to describe, easy to do...
- Only one program is written, executed in batch on all processors.
- Different processors are autonomous; there is no manager.
- The dominant programming model for large machines.

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.

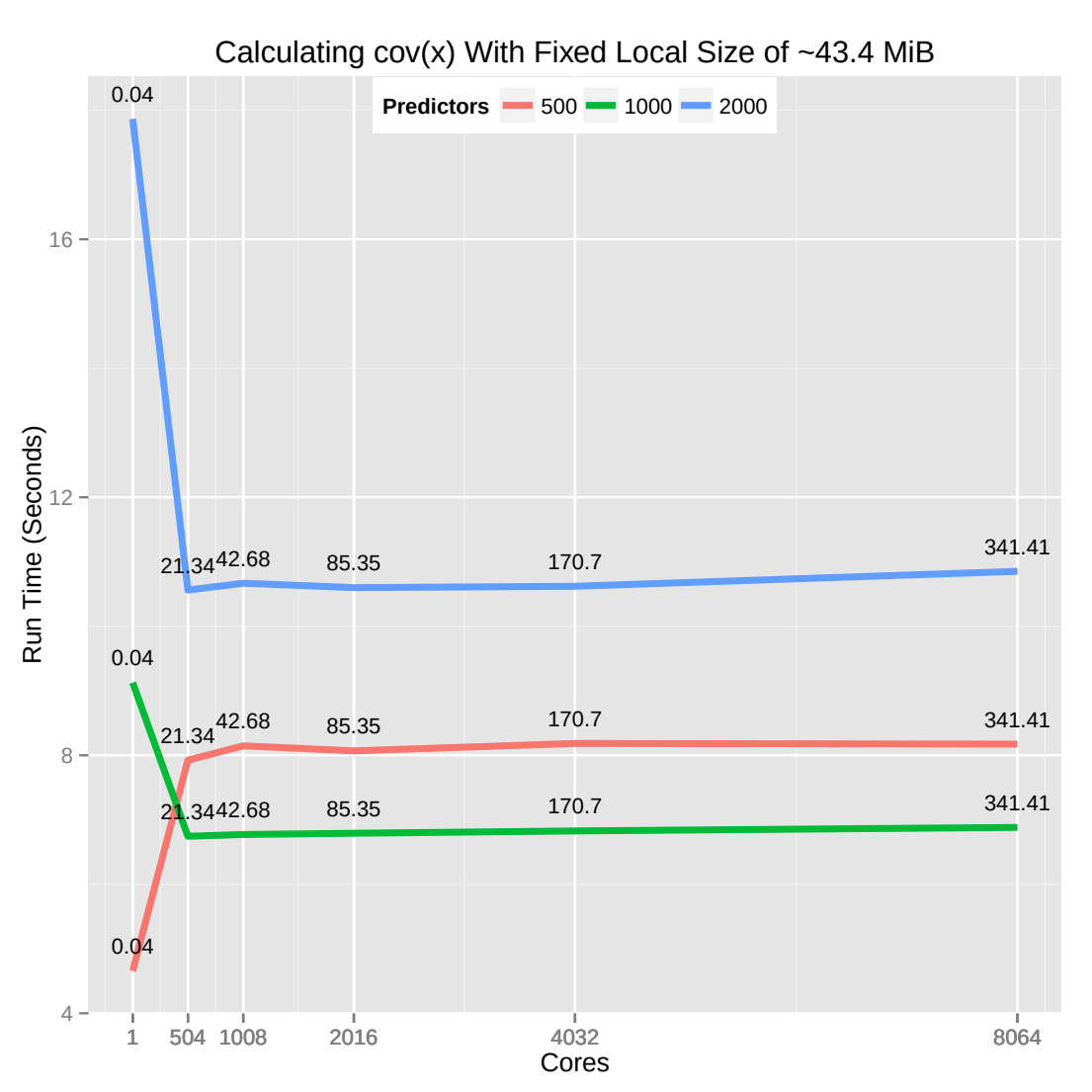
Benchmark Data

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

```
1 x <- ddmatrix("rnorm", nrow=n, ncol=p, mean=mean, sd=sd)
2
3 cov.x <- cov(x)
```

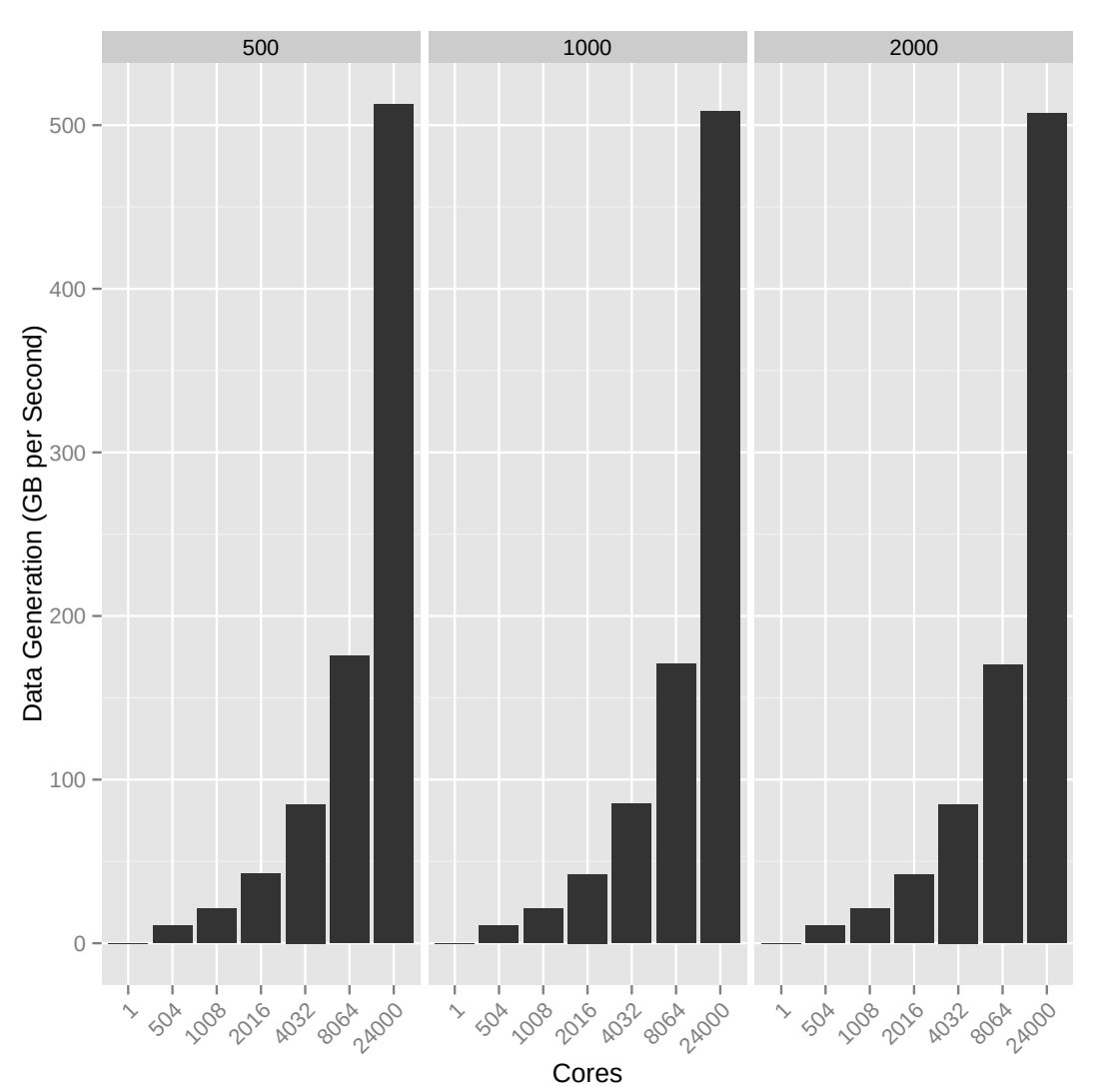
cov()


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

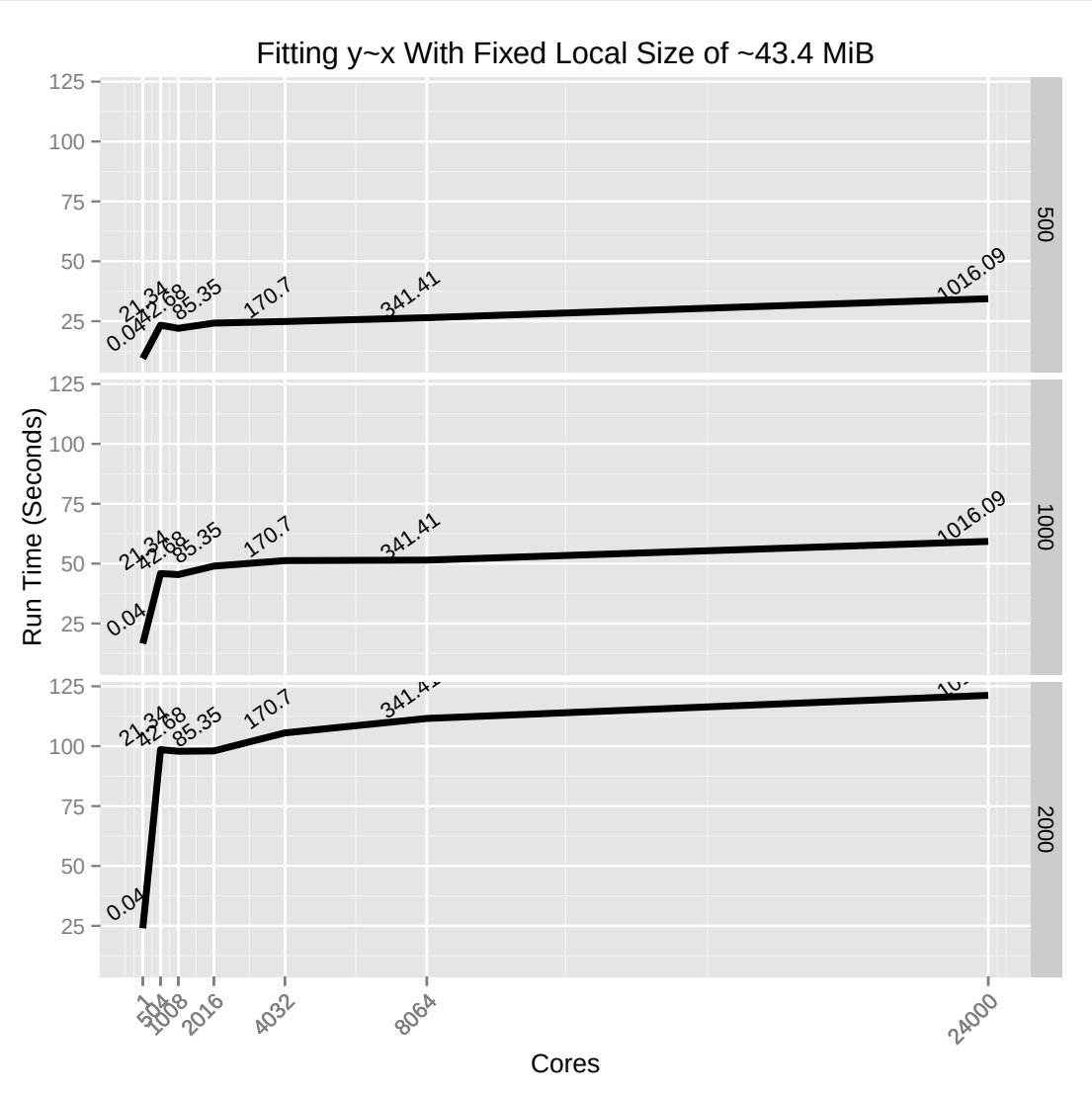
Linear Model Code

```
1 x <- ddmatrix("rnorm", nrow=n, ncol=p, mean=mean, sd=sd)
2 beta_true <- ddmatrix("runif", nrow=p, ncol=1)
3
4 y <- x %*% beta_true
5
6 beta_est <- lm.fit(x=x, y=y)$coefficients
```

Data Generation



lm.fit()


Fitting y~x With Fixed Local Size of ~43.4 MiB
Run Time (Seconds)
125
100
75
50
25
500
1000
2000
0.04
21.34
42.68
85.35
170.7
341.41
1016.09
1
504
1008
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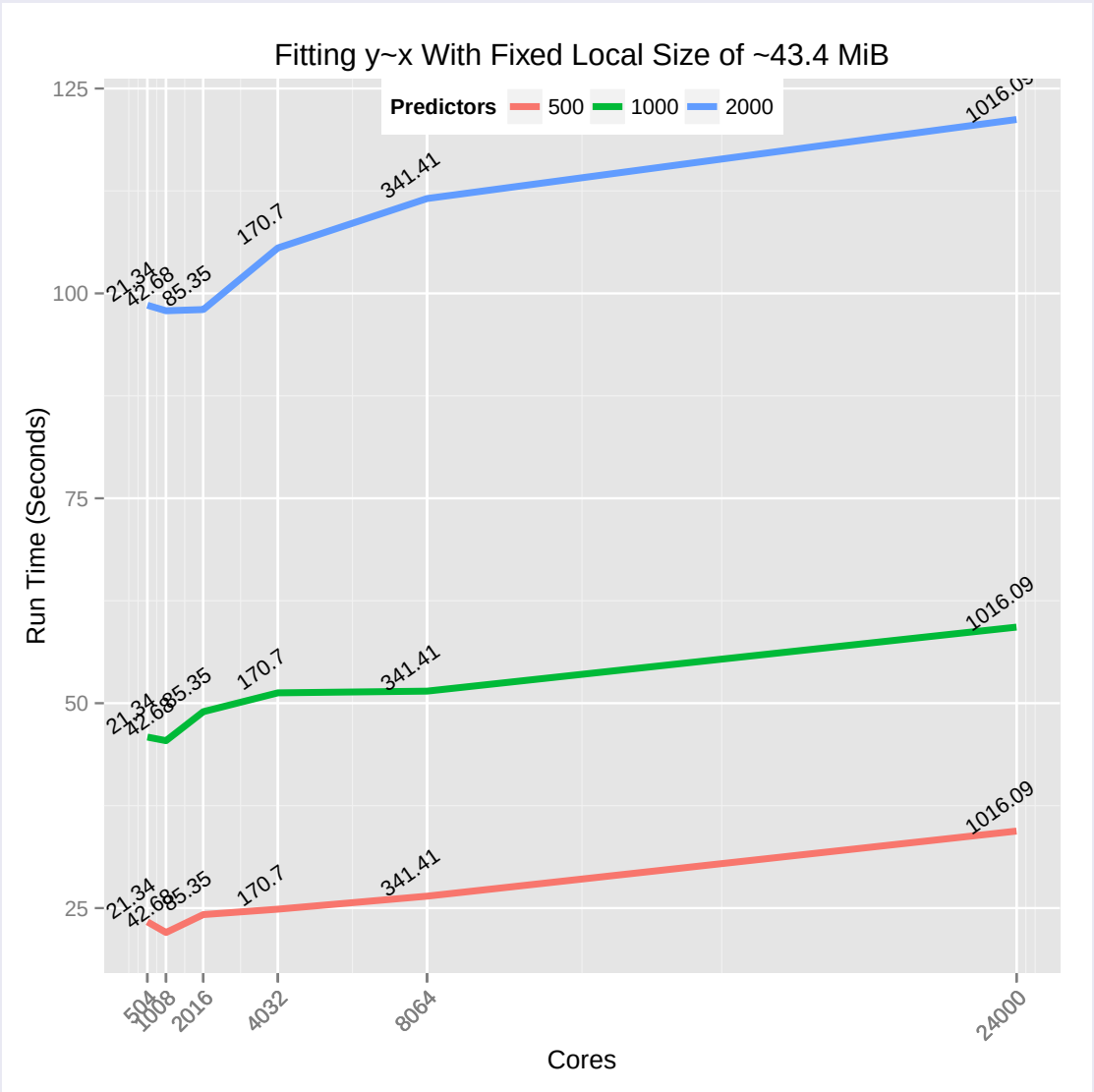
Cores

lm.fit()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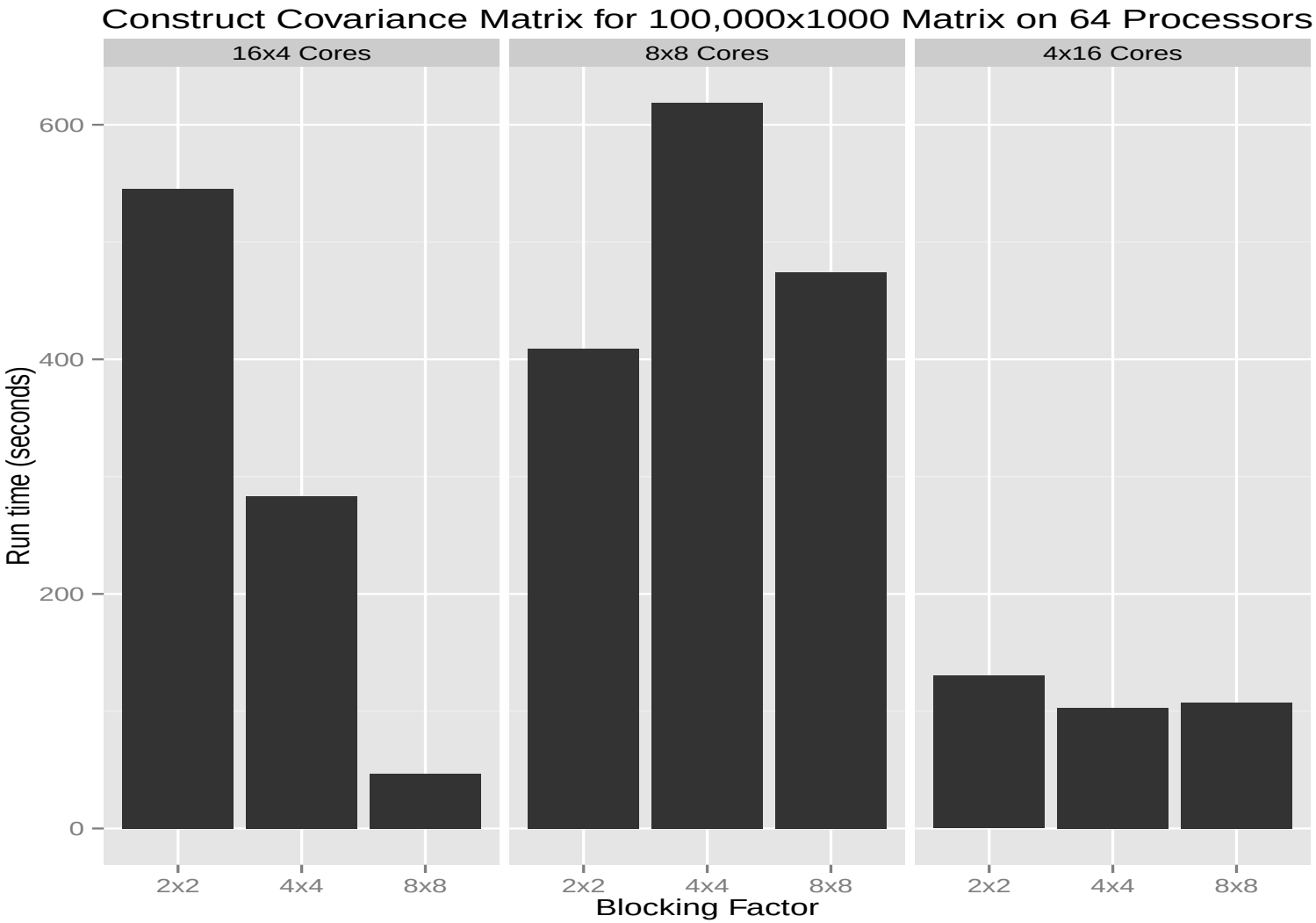
Cores

Contents

Challenges

- Perceptions.
- Library loading.
- Profiling.

Covariance Revisited: Distributed Data Parameter Calibration



Tutorials

- SC13, November 17-22, Denver, Colorado, USA

Invited Talks

- IASC, Aug 22-23, Seoul
- World Statistics Congress, August 25-30, Hong Kong

Thanks for coming!

Questions?

Be sure to stick around for the tutorial