High Performance Computing with R

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Tutorial Structure

1. (45 Minutes) Basics: Intro, debugging, profiling, benchmarking.
2. (15 Minutes) Exercises

3. (45 Minutes) Improving R Code: compilers, vectorization, loops, ...
4. (30 Minutes) Exercises + Break

5. (45 Minutes) Interfacing to Compiled Code
6. (15 Minutes) Exercises

7. (45 Minutes) Parallelism

Tutorial Goals

We hope to introduce you to:

1. Basic debugging.
2. Evaluating the performance of R code.
3. Some R best practices to help with performance.
4. Why and how to interface R to C++.
5. Basics of parallelism in R.

Exercises

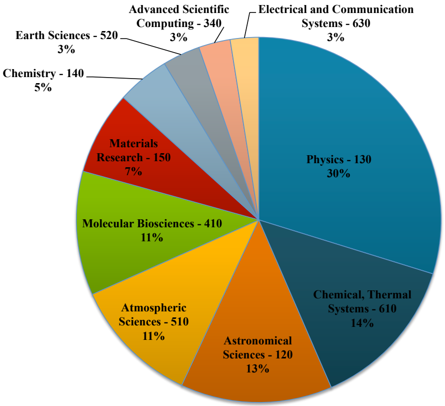
Each section has a complement of exercises to give hands-on reinforcement of ideas introduced in the lecture.

1. More exercises are given than you have time to complete.
2. Later exercises are more difficult than earlier ones.
3. Some exercises require use of things not explicitly shown in lecture; look through the documentation mentioned in the slides to find the information you need.

National Institute for Computational Sciences
University of Tennessee & ORNL partnership

- NICS is an NSF HPC center established in 2007
  - Takes advantage of the strengths of UT and ORNL
- Series of computers that culminated in a 1.17 Petaflop system in Jan 2011
  - First Academic Petaflop: Kraken

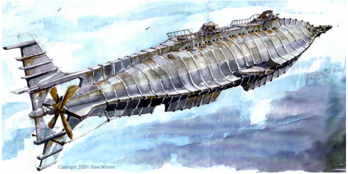
Kraken Actual Usage by Discipline (Aug'12) 79.2M hours



NICS Now...

- Growing our Data Sciences
- Collaborating with industry to advance several fields
- Supply NSF cycles through Darter, Beacon, and Nautilus

Nautilus SGI UltraViolet specs



Compute processor type	Intel ~2.0 GHz Nehalem
Compute cores	1024
Compute sockets (nodes)	128 oct-core
Memory per core	**4 GB**
Total memory	4 TB (SMP)
Accelerators	8 NVIDIA Fermi GPUs
Peak system performance	10 TF
Interconnect topology	NUMAlink5
Parallel file system space	1 PB (Lustre)
Parallel file system peak performance	30 GB/s

Newest Resources

Conventional Intel Processors

Darter Cray XC30 Supercomputer Peak Performance: 248.9 TFLOP/s	
Compute Nodes	748
CPU model	Intel Xeon E5-2670
CPUs per node	2 8-core, 2.6GHz
RAM per node	16 GB
Interconnect	Cray Aries Dragonfly

Hosted Accelerators: Intel MICs

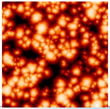
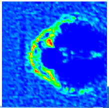
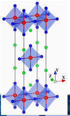
Beacon Cray Xtreme-X Supercomputer Peak Performance: 210.1 TFLOP/s	
Compute Nodes	48
CPU model	Intel Xeon E5-2670
CPUs per node	2 8-core, 2.6GHz
RAM per node	256 GB
SSD per node	2 x 480 GB (RAID 0)
Intel® Xeon Phi Coprocessors per node	4 x 5110P 60-core, 1.053GHz 8 GB GDDR5 RAM
Interconnect	FDR InfiniBand Fat Tree

#1 on Green500

XSEDE

Extreme Science and Engineering Discovery Environment

- Extreme Science and Engineering Discovery Environment
- Follow on NSF project to TeraGrid in 2012
- Centers operate machines, and XSEDE provides seamless infrastructure for allocations, access, and training
- Researchers propose resource use through XRAS
- Supports thousands of scientists in fields such as:
  - Chemistry
  - Bioinformatics
  - Materials Science
  - Data Sciences

XSEDE Allocations

- Want to use XSEDE resources to teach a class?
  - https://portal.xsede.org/allocations-overview#types-education
- Just looking to try out a larger resource or a special resource your campus doesn't have?
  - https://portal.xsede.org/allocations-overview#types-startup

XSEDE Allocations

- See a Campus Champion
  - https://www.xsede.org/current-champions
- Ready to scale up your research?
  - https://portal.xsede.org/allocations-overview#types-research

More “helpful” resources

xsede.org→User Services

- Resources available at each Service Provider
  - User Guides describing memory, number of CPUs, file systems, etc.
  - Storage facilities
  - Software (Comprehensive Search)
- Training: portal.xsede.org → Training
  - Course Calendar
  - On-line training
  - Certifications
- Get face-to-face help from XSEDE experts at your institution; contact your local Campus Champions.
- Extended Collaborative Support (formerly known as Advanced User Support (AUSS))

Part I

Basics

1 Introduction

- A 5 Minute Introduction to R
- R is for Lunatics
- R Resources
- Summary

Types

- `logical` ("boolean")
- `integer` (32-bit int)
- `numeric` (double)
- `complex` (double complex)
- `character` (string)

Happy Opposite Day!

```r
T
# [1] TRUE
F
# [1] FALSE

T <- FALSE
F <- TRUE

T
# [1] FALSE
F
# [1] TRUE
```

Package or Library?

- I wrote a library.
- I put that library into a package.
- I installed the package ... into a library.
- I load the package with `library()` ???

BOOM

R: A Language for Lunatics

"*R is a shockingly dreadful language for an exceptionally useful data analysis environment.*" — Tim Smith, from **aRrgh: a newcomer's (angry) guide to R**.

But you can't deny its popularity!

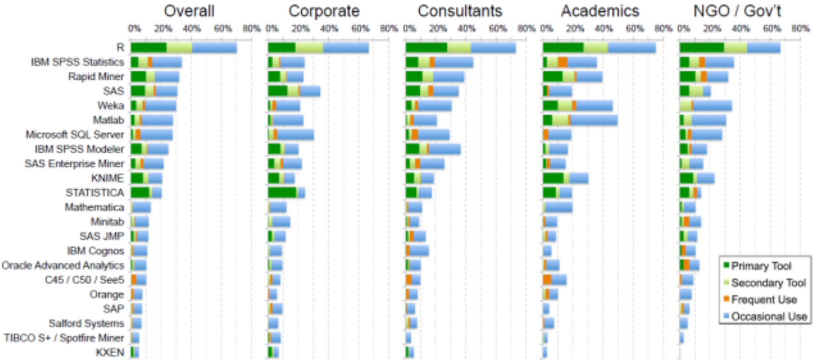
IEEE Spectrum's 2014 Ranking of Programming Languages

Language Rank	Types	Spectrum Ranking
1. Java		100.0
2. C		99.3
3. C++		95.5
4. Python		93.4
5. C#		92.4
6. PHP		84.7
7. Javascript		84.4
8. Ruby		78.8
9. R		74.2
10. MATLAB		72.9

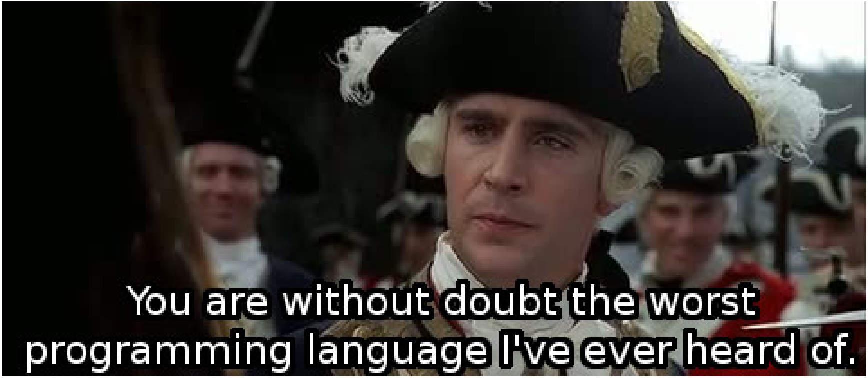
See:

http://spectrum.ieee.org/static/interactive-the-top-programming-languages#index

Top Data Analysis Tool



See: http://www.rexeranalytics.com/Data-Miner-Survey-2013-Intro.html


You are without doubt the worst
programming language I've ever heard of.


R
But you HAVE heard of me!

Why use R at all?

- Most diverse set of statistical methods available.
- Rapid prototyping.
- CRAN (and increasingly GitHub) packages.
- *Awesome* community.
- Syntax is designed for analysis of data.

Resources for Learning R

- *The Art of R Programming* by Norm Matloff: http://nostarch.com/artofr.htm
- *An Introduction to R* by Venables, Smith, and the R Core Team: http://cran.r-project.org/doc/manuals/R-intro.pdf
- *The R Inferno* by Patrick Burns: http://www.burns-stat.com/pages/Tutor/R_inferno.pdf
- Mathesaurus: http://mathesaurus.sourceforge.net/
- R programming for those coming from other languages: http://www.johndcook.com/R_language_for_programmers.html
- *aRrgh: a newcomer's (angry) guide to R*, by Tim Smith and Kevin Ushey: http://tim-smith.us/arrgh/

Other Invaluable Resources

- *R Installation and Administration*: http://cran.r-project.org/doc/manuals/R-admin.html
- *Task Views*: http://cran.at.r-project.org/web/views
- *Writing R Extensions*: http://cran.r-project.org/doc/manuals/R-exts.html
- Mailing list archives: http://tolstoy.newcastle.edu.au/R/
- The `[R]` stackoverflow tag.
- The `#rstats` hastag on Twitter.

Summary

- R is more data analysis package than programming language.
- But you can't deny its popularity!

2 Debugging

Debugging R Code

- Very broad topic ...
- We'll hit the highlights.
- For more examples, see:
  `cran.r-project.org/doc/manuals/R-exts.html#Debugging`

Object Inspection Tools

- `print()`
- `str()`
- `unclass()`

Object Inspection Tools: `print()`

Basic printing:

```
> x <- matrix(1:10, nrow=2)
> print(x)
     [,1] [,2] [,3] [,4] [,5]
[1,]    1    3    5    7    9
[2,]    2    4    6    8   10
> x
     [,1] [,2] [,3] [,4] [,5]
[1,]    1    3    5    7    9
[2,]    2    4    6    8   10
```

Object Inspection Tools: `str()`

Examining the **<u>str</u>**ucture of an R object:

```
> x <- matrix(1:10, nrow=2)
> str(x)
 int [1:2, 1:5] 1 2 3 4 5 6 7 8 9 10
```

Object Inspection Tools: unclass()

Exposing all data with unclass():

```
df <- data.frame(x=rnorm(10), y=rnorm(10))
mdl <- lm(y~x, data=df) ### That's a "tilde" character

mdl
print(mdl)

str(mdl)

unclass(mdl)
```

Try it!

The R Debugger

- `debug()`
- `debugonce()`
- `undebug()`

Using The R Debugger

1. Declare function to be debugged: `debug(foo)`
2. Call function: `foo(arg1, arg2, ...)`
   - next: `Enter` or `n` followed by `Enter`.
   - break: Halt execution and exit debugging: `Q`.
   - exit: Continue execution and exit debugging: `c`.
3. Call `undebug()` to stop debugging

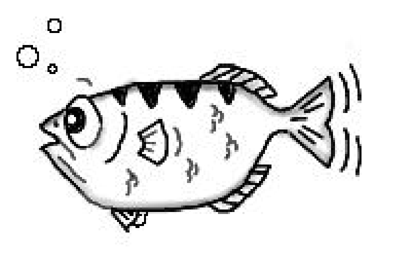
Using the Debugger

Example Debugger Interaction

```
> f <- function(x){y <- z+1;z <- y*2;z}
> f(1)
Error in f(1) : object 'z' not found
> debug(f)
> f(1)
debugging in: f(1)
debug at #1: {
    y <- z + 1
    z <- y * 2
    z
}
Browse[2]>
debug at #1: y <- z + 1
Browse[2]>
Error in f(1) : object 'z' not found
>
```

Debugging Compiled Code

- Reasonably easy to use gdb and Valgrind (from command line).
- gdb — The GNU Debugger; general purpose debugging.
- Valgrind — Memory debugger.
- For gdb, start R interactively.
- For Valgrind, need a batch script.



Debugging with gdb

Suppose we have:

- R function: `fooR()`
- Calls the C function: `fooC()`

We can debug `fooC()` via gdb by executing the following from a shell:

```
R -d gdb
b fooC
signal 0
fooR(10)
```

Debugging with Valgrind

Put the R code you wish to profile in `myscript.r` and execute the following from a shell:

```
R -d "valgrind --tool=memcheck --leak-check=full" --vanilla <
    myscript.r
```

2 Debugging

- Debugging R Code
- The R Debugger
- Debugging Compiled Code Called by R Code
- Summary

Summary

- R has sophisticated debugging utilities for dealing with buggy R code. (`debug()`, `str()`, ...).
- Using gdb is awkward, but possible.
- Using Valgrind is straight-forward.

3 Profiling
- Why Profile?
- Profiling R Code
- Advanced R Profiling
- Summary

Performance and Accuracy

Sometimes $\pi = 3.14$ is (a) infinitely faster than the "correct" answer and (b) the difference between the "correct" and the "wrong" answer is meaningless. . . . The thing is, some specious value of "correctness" is often irrelevant because it doesn't matter. While performance almost always matters. And I absolutely detest the fact that people so often dismiss performance concerns so readily.

— Linus Torvalds, August 8, 2008

Why Profile?

- Because performance matters.
- Bad practices scale up!
- Your bottlenecks may surprise you.
- Because R is dumb.
- R users claim to be data people. . . so act like it!

Compilers often correct bad behavior...

A Really Dumb Loop

```c
int main(){
    int x, i;
    for (i=0; i<10; i++)
        x = 1;
    return 0;
}
```

clang -O3 -S example.c

```
main:
        .cfi_startproc
# BB#0:
        xorl    %eax,
            %eax
        ret
```

clang -S example.c

```
main:
        .cfi_startproc
# BB#0:
        movl    $0, -4(%rsp)
        movl    $0, -12(%rsp)
.LBB0_1:
        cmpl    $10, -12(%rsp)
        jge     .LBB0_4
# BB#2:
        movl    $1, -8(%rsp)
# BB#3:
        movl    -12(%rsp), %eax
        addl    $1, %eax
        movl    %eax, -12(%rsp)
        jmp     .LBB0_1
.LBB0_4:
        movl    $0, %eax
        ret
```

R will not!

Dumb Loop

```
for (i in 1:n){
  tA <- t(A)
  Y <- tA %*% Q
  Q <- qr.Q(qr(Y))
  Y <- A %*% Q
  Q <- qr.Q(qr(Y))
}

Q
```

Better Loop

```
tA <- t(A)

for (i in 1:n){
  Y <- tA %*% Q
  Q <- qr.Q(qr(Y))
  Y <- A %*% Q
  Q <- qr.Q(qr(Y))
}

Q
```

Example from a Real R Package

Exerpt from Original function

```
while(i<=N){
  for(j in 1:i){
     d.k <- as.matrix(x)[l==j,l==j]
       ...
```

Exerpt from Modified function

```
x.mat <- as.matrix(x)

while(i<=N){
  for(j in 1:i){
     d.k <- x.mat[l==j,l==j]
       ...
```

By changing just 1 line of code, performance of the main method improved by **over 350%**!

Some Thoughts

- R is slow.
- Bad programmers are slower.
- R can't fix bad programming.

Timings

Getting simple timings as a basic measure of performance is easy, and valuable.

- `system.time()` — timing blocks of code.
- `Rprof()` — timing execution of R functions.
- `Rprofmem()` — reporting memory allocation in R .
- `tracemem()` — detect when a copy of an R object is created.

Performance Profiling Tools: system.time()

system.time() is a basic R utility for timing expressions

```r
x <- matrix(rnorm(20000*750), nrow=20000, ncol=750)

system.time(t(x) %*% x)
#    user  system elapsed
#   2.187   0.032   2.324

system.time(crossprod(x))
#    user  system elapsed
#   1.009   0.003   1.019

system.time(cov(x))
#    user  system elapsed
#   6.264   0.026   6.338
```

Performance Profiling Tools: `system.time()`

Put more complicated expressions inside of brackets:

```r
x <- matrix(rnorm(20000*750), nrow=20000, ncol=750)

system.time({
  y <- x+1
  z <- y*2
})
#    user  system elapsed
#   0.057   0.032   0.089
```

Performance Profiling Tools: Rprof()

```r
Rprof(filename="Rprof.out", append=FALSE, interval=0.02,
  memory.profiling=FALSE, gc.profiling=FALSE,
  line.profiling=FALSE, numfiles=100L, bufsize=10000L)
```


NO FAIR!
YOU CHANGED THE OUTCOME BY MEASURING IT

Performance Profiling Tools: Rprof()

```r
x <- matrix(rnorm(10000*250), nrow=10000, ncol=250)

Rprof()
invisible(prcomp(x))
Rprof(NULL)

summaryRprof()

Rprof(interval=.99)
invisible(prcomp(x))
Rprof(NULL)

summaryRprof()
```

Performance Profiling Tools: Rprof()

```
$by.self
                  self.time self.pct total.time total.pct
"La.svd"               0.68    69.39       0.72     73.47
"%*%"                  0.12    12.24       0.12     12.24
"aperm.default"        0.04     4.08       0.04      4.08
"array"                0.04     4.08       0.04      4.08
"matrix"               0.04     4.08       0.04      4.08
"sweep"                0.02     2.04       0.10     10.20
### output truncated by presenter

$by.total
                   total.time total.pct self.time self.pct
"prcomp"                 0.98    100.00      0.00     0.00
"prcomp.default"         0.98    100.00      0.00     0.00
"svd"                    0.76     77.55      0.00     0.00
"La.svd"                 0.72     73.47      0.68    69.39
### output truncated by presenter

$sample.interval
[1] 0.02

$sampling.time
[1] 0.98
```

Performance Profiling Tools: Rprof()

```
$by.self
[1] self.time  self.pct   total.time total.pct
<0 rows> (or 0-length row.names)

$by.total
[1] total.time total.pct  self.time  self.pct
<0 rows> (or 0-length row.names)

$sample.interval
[1] 0.99

$sampling.time
[1] 0
```

3 Profiling

- Why Profile?
- Profiling R Code
- Advanced R Profiling
- Summary

Other Profiling Tools

- perf, PAPI
- fpmpi, mpiP, TAU
- pbdPROF
- pbdPAPI

Profiling MPI Codes with **pbdPROF**

1. Rebuild pbdR packages

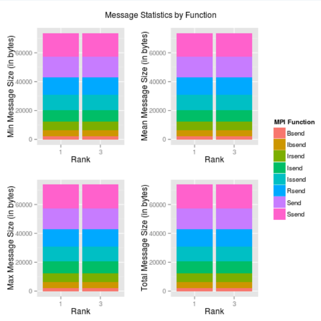
```
R CMD INSTALL pbdMPI_0.2-1.tar.gz \
    --configure-args= \
    "--enable-pbdPROF"
```

2. Run code

```
mpirun -np 64 Rscript my_script.R
```

3. Analyze results

```r
library(pbdPROF)
prof <- read.prof( "output.mpiP")
plot(prof, plot.type="messages2")
```



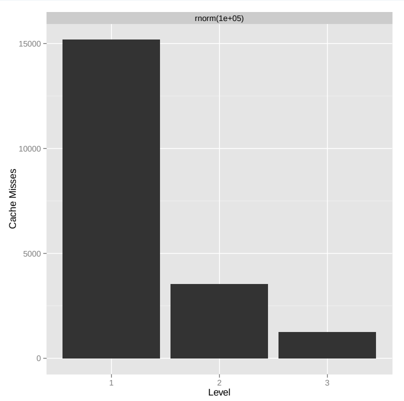
Profiling with **pbdPAPI**

- Bindings for Performance Application Programming Interface (PAPI)
- Gathers detailed hardware counter data.
- High and low level interfaces

Function	Description of Measurement
`system.flips()`	Time, floating point instructions, and Mflips
`system.flops()`	Time, floating point operations, and Mflops
`system.cache()`	Cache misses, hits, accesses, and reads
`system.epc()`	Events per cycle
`system.idle()`	Idle cycles
`system.cpuormem()`	CPU or RAM bound*
`system.utilization()`	CPU utilization*

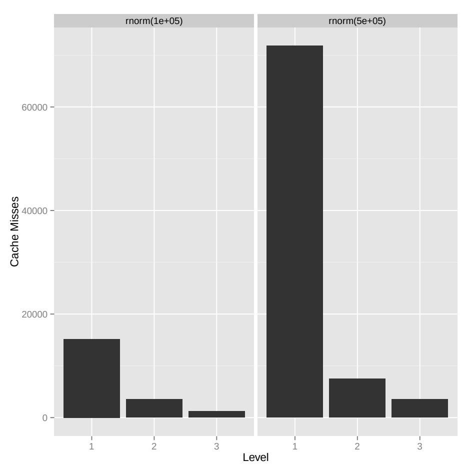
Profiling with **pbdPAPI**

```r
x <- system.cache(rnorm(1e5), type="miss")
x
# L1 Cache Misses: 15186
# L2 Cache Misses: 3550
# L3 Cache Misses: 1241

plot(x)
```



Profiling with **pbdPAPI**

```r
y <- system.cache(rnorm(5e5), type="miss")

plot(x, y)
```



pbdPAPI

To learn more about pbdPAPI, see:

- Guide to the pbdPAPI Package
- Advanced R Profiling with pbdPAPI
- Cache Rules Everything Around Me

Summary

- *Profile, profile, profile.*
- Use `system.time()` to get a general sense of a method.
- Use `Rprof()` for more detailed profiling.
- Other tools exist for more hardcore applications (e.g., **pbdPAPI** and **pbdPROF**).

Exercises

Part II

Improving R Performance

Benchmarking

- There's *a lot* that goes on when executing an R funciton.
- Symbol lookup, creating the abstract syntax tree, creating promises for arguments, argument checking, creating environments, ...
- Executing a second time can have dramatically different performance over the first execution.
- Benchmarking several methods fairly requires some care.

Benchmarking tools: rbenchmark

rbenchmark is a simple package that easily benchmarks different functions:

```
x <- matrix(rnorm(10000*500), nrow=10000, ncol=500)

f <- function(x) t(x) %*% x
g <- function(x) crossprod(x)

library(rbenchmark)
benchmark(f(x), g(x), columns=c("test", "replications",
    "elapsed", "relative"))

#   test replications elapsed relative
# 1 f(x)          100  13.679    3.588
# 2 g(x)          100   3.812    1.000
```

Benchmarking tools: microbenchmark

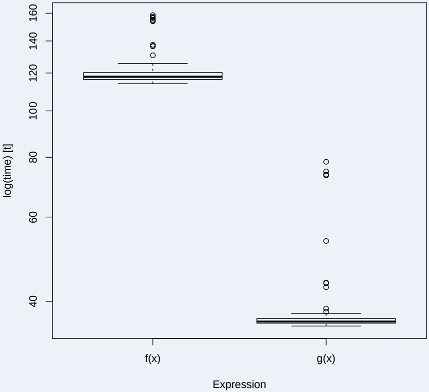
microbenchmark is a separate package with a slightly different philosophy:

```
x <- matrix(rnorm(10000*500), nrow=10000, ncol=500)

f <- function(x) t(x) %*% x
g <- function(x) crossprod(x)

library(microbenchmark)
microbenchmark(f(x), g(x), unit="s")

# Unit: seconds
#  expr         min          lq        mean      median          uq
          max neval
#  f(x) 0.11418617 0.11647517 0.12258556 0.11754302 0.12058145
    0.17292507   100
#  g(x) 0.03542552 0.03613772 0.03884497 0.03668231 0.03740173
    0.07478309   100
```

Benchmarking tools: microbenchmark

I generally prefer **rbenchmark**, but the built-in plots for **microbenchmark** are nice:

```
bench <- microbenchmark(f(x), g(x), unit="s")

boxplot(bench)
```



4 Benchmarking
- Benchmarking
- Summary

Summary

- Don't just time 1 evaluation to compare 2 methods.
- You could write the stuff yourself easily enough...
- But **rbenchmark** and **microbenchmark** already exist and work very well.

Better Compiler

- GNU (gcc/gfortran) and clang/gfortran are free and will compile anything, but don't produce the fastest binaries.
- Don't even bother with MSVC.
- Intel icc is very fast on intel hardware.

$$\text{Better compiler} \implies \text{Faster R}$$

Compiling R with icc and ifort

- Faster, but not painless.
- Requires Intel Composer suite license ($$$).
- Improvements are most visible on Intel hardware.
- See Intel's help pages for details.

The Compiler Package

- Released in 2011 (Tierney)
- Bytecode: sort of like machine code for interpreters...
- Improves R code speed by 2-5% generally.
- Does best on loops.

Bytecode Compilation

- Non-core packages not (bytecode) compiled by default.
- "Base" and "recommended" (core) packages are.
- Downsides:
  - (slightly) larger install size
  - (much!) longer install process
  - doesn't fix bad code
- Upsides: slightly faster.

Compiling a Function

```
test <- function(x) x+1
test
# function(x) x+1

library(compiler)

test <- cmpfun(test)
test
# function(x) x+1
# <bytecode: 0x38c86c8>

disassemble(test)
# list(.Code, list(7L, GETFUN.OP, 1L, MAKEPROM.OP, 2L,
    PUSHCONSTARG.OP,
#     3L, CALL.OP, 0L, RETURN.OP), list(x + 1, `+`, list(.Code,
#     list(7L, GETVAR.OP, 0L, RETURN.OP), list(x)), 1))
```

Compiling Packages

From R

```r
install.packages("my_package", type="source",
    INSTALL_opts="--byte-compile")
```

From The Shell

```sh
export R_COMPILE_PKGS=1
R CMD INSTALL my_package.tar.gz
```

Or add the line: `ByteCompile: yes` to the package's `DESCRIPTION` file.

The Compiler: How much does it help *really*?

```r
f <- function(n) for (i in 1:n) 2*(3+4)


library(compiler)
f_comp <- cmpfun(f)


library(rbenchmark)

n <- 100000
benchmark(f(n), f_comp(n), columns=c("test", "replications",
    "elapsed", "relative"),
order="relative")
#         test replications elapsed relative
# 2 f_comp(n)          100   2.604    1.000
# 1       f(n)          100   2.845    1.093
```

The Compiler: How much does it help *really*?

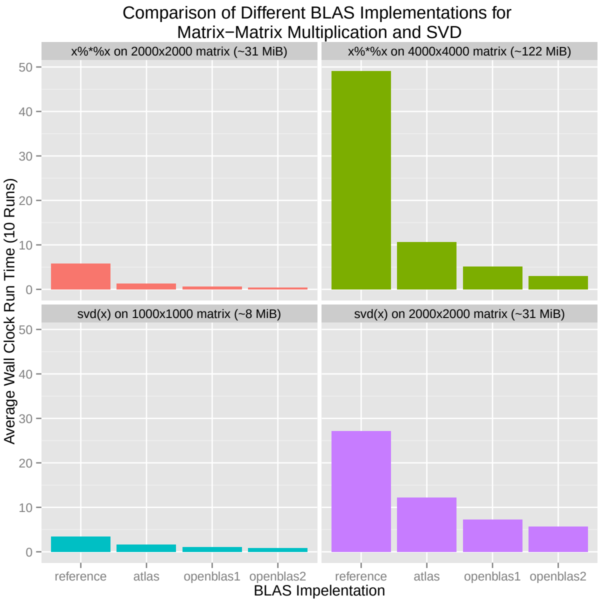
```r
g <- function(n)
{
  x <- matrix(runif(n*n), nrow=n, ncol=n)
  min(colSums(x))
}


library(compiler)
g_comp <- cmpfun(g)


library(rbenchmark)

n <- 1000
benchmark(g(n), g_comp(n), columns=c("test", "replications",
    "elapsed", "relative"),
order="relative")
#          test replications elapsed relative
# 2 g_comp(n)          100   6.854    1.000
# 1      g(n)          100   6.860    1.001
```

The BLAS

- Basic Linear Algebra Subprograms.
- Basic numeric matrix operations.
- Used to compute matrix factorizations (LAPACK).
- Used in linear algebra and many statistical operations.
- Different implementations available.
- Several multithreaded BLAS libraries exist.

Benchmark

```r
set.seed(1234)
m <- 2000
n <- 2000
x <- matrix(
  rnorm(m*n),
  m, n)

object.size(x)

library(rbenchmark)

benchmark(x%*%x)
benchmark(svd(x))
```



Using Parallel BLAS

- See the R Installation and Administration manual for info.
- **Warning:** doesn't always play nice with the **parallel** package!

5 Free Improvements
- Building R with a Different Compiler
- The Bytecode Compiler
- Choice of BLAS Library
- Summary

Summary

- Compiling R itself with a different compiler can improve performance, but is non-trivial.
- The compiler package offers small, but free speedup.
- The (bytecode) compiler works best on loops.

6 Writing Better R Code

- Loops
- Ply Functions
- Vectorization
- Loops, Plys, and Vectorization
- Summary

Loops

- `for`
- `while`
- No `goto`'s or `do while`'s.
- They're *really* slow.

Loops: Best Practices

- *Profile, profile, profile.*
- Mostly try to avoid.
- Evaluate practicality of rewrite (plys, vectorization, compiled code)
- Always preallocate!

Loops 1

```r
square_loop_noinit <- function(n){
  x <- c()
  for (i in 1:n){
    x <- c(x, i^2)
  }

  x
}


square_loop_withinit <- function(n){
  x <- integer(n)
  for (i in 1:n){
    x[i] <- i^2
  }

  x
}
```

Loops 2

```r
library(rbenchmark)
n <- 1000

benchmark(square_loop_noinit(n), square_loop_withinit(n))
#                      test replications elapsed relative
# 1   square_loop_noinit(n)          100   0.257    2.596
# 2 square_loop_withinit(n)          100   0.099    1.000
```

6 Writing Better R Code

- Loops
- Ply Functions
- Vectorization
- Loops, Plys, and Vectorization
- Summary

"Ply" Functions

- R has functions that apply other functions to data.
- In a nutshell: loop sugar.
- Typical *ply's:
  - `apply()`: apply function over matrix "margin(s)".
  - `lapply()`: apply function over list/vector.
  - `mapply()`: apply function over multiple lists/vectors.
  - `sapply()`: same as `lapply()`, but (possibly) nicer output.
  - Plus some other mostly irrelevant ones.
- Also `Map()` and `Reduce()`.

Ply Examples: apply()

```r
x <- matrix(1:10, 2)

x
#       [,1] [,2] [,3] [,4] [,5]
# [1,]     1    3    5    7    9
# [2,]     2    4    6    8   10

apply(X=x, MARGIN=1, FUN=sum)
# [1] 25 30

apply(X=x, MARGIN=2, FUN=sum)
# [1]  3  7 11 15 19

apply(X=x, MARGIN=1:2, FUN=sum)
#       [,1] [,2] [,3] [,4] [,5]
# [1,]     1    3    5    7    9
# [2,]     2    4    6    8   10
```

Ply Examples: lapply() and sapply()

```r
lapply(1:4, sqrt)
# [[1]]
# [1] 1
#
# [[2]]
# [1] 1.414214
#
# [[3]]
# [1] 1.732051
#
# [[4]]
# [1] 2

sapply(1:4, sqrt)
# [1] 1.000000 1.414214 1.732051 2.000000
```

Transforming Loops Into Ply's

```r
vec <- numeric(n)
for (i in 1:n){
  vec[i] <- my_function(i)
}
```

Becomes:

```r
sapply(1:n, my_function)
```

Ply's: Best Practices

- Most ply's are just shorthand/higher expressions of loops.
- Generally not much faster (if at all), especially with the compiler.
- Thinking in terms of `lapply()` can be useful however...

Ply's: Best Practices

- With ply's and lambdas, can do some fiendishly crafty things.
- But don't go crazy...

```
cat(sapply(letters, function(a) sapply(letters, function(b)
    sapply(letters, function(c) sapply(letters, function(d)
    paste(a, b, c, d, letters, "\n", sep=""))))))
```

6 Writing Better R Code

- Loops
- Ply Functions
- Vectorization
- Loops, Plys, and Vectorization
- Summary

Vectorization

- `x+y`
- `x[, 1] <- 0`
- `rnorm(1000)`

Vectorization

- Same in R as in other high-level languages (Matlab, Python, . . .).
- Idea: use pre-existing compiled kernels to avoid interpreter overhead.
- Much faster than loops and plys.

```r
ply <- function(x) lapply(rep(1, 1000), rnorm)
vec <- function(x) rnorm(1000)

library(rbenchmark)
benchmark(ply(x), vec(x))
#     test replications elapsed relative
# 1 ply(x)          100   0.348   38.667
# 2 vec(x)          100   0.009    1.000
```

Vectorization Best Practices

- Vectorize if at all possible.
- Note that this consumes potentially a lot of memory!

Putting It All Together

- Loops are slow.
- `apply()`, `Reduce()` are just `for` loops.
- `Map()`, `lapply()`, `sapply()`, `mapply()` (and most other core ones) are *not* `for` loops.
- *Ply functions are not vectorized*.
- Vectorization is fastest, but often needs lots of memory.

Squares

Let's compute the square of the numbers 1–100000, using

- `for` loop without preallocation
- `for` loop with preallocation
- `sapply()`
- vectorization

Squares

```r
square_sapply <- function(n) sapply(1:n, function(i) i^2)

square_vec <- function(n) (1:n)*(1:n)
```

```r
library(rbenchmark)
n <- 100000

benchmark(square_loop_noinit(n), square_loop_withinit(n),
    square_sapply(n), square_vec(n))
#                      test replications elapsed relative
# 1   square_loop_noinit(n)          100  17.296 2470.857
# 2 square_loop_withinit(n)          100   0.933  133.286
# 3        square_sapply(n)          100   1.218  174.000
# 4           square_vec(n)          100   0.007    1.000
```

6 Writing Better R Code

Summary

- Pre-allocate your data in loops.
- Vectorize when you can.
- Try a ply function when you can't.

Exercises

Part III

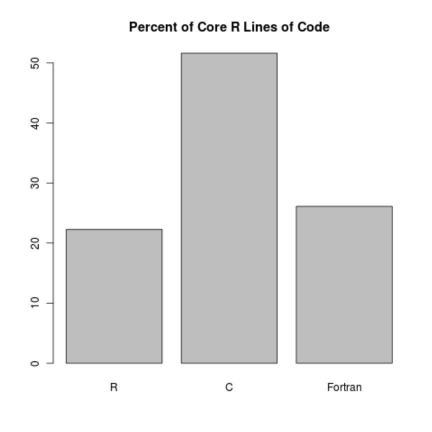
Interfacing to Compiled Code

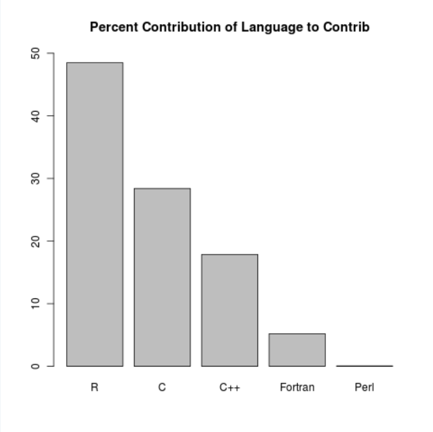
7 Introduction to Rcpp

- Foreign Language Interfaces
- What is Rcpp?
- Documentation and Help

What Language is R Written In?

- R is mostly a C program
- R extensions are mostly R programs





Foreign Language Interfaces

- C/C++: `.Call()`, `.C()` (deprecated)
- Fortran: `.Call()`, `.Fortran()` (deprecated)
- Java: rJava package
- Python: rPython package
- ...

For the remainder, we will focus on C++ via Rcpp.

7 Introduction to Rcpp
- Foreign Language Interfaces
- What is Rcpp?
- Documentation and Help

What Rcpp **is**

- R interface to compiled code.
- Package ecosystem (Rcpp, RcppArmadillo, RcppEigen, . . .).
- Utilities to make writing C++ more convenient for R users.
- **A tool which requires C++ knowledge to effectively utilize.**
- GPL licensed (like R).

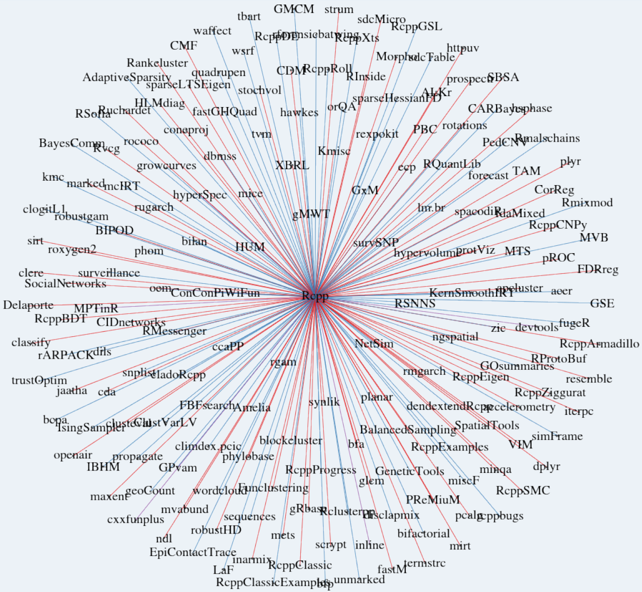
What Rcpp **is not**

- Magic.
- Automatic R-to-C++ converter.
- A way around having to learn C++.
- A tool to make existing R functionality faster (unless you rewrite it!).
- As easy to use as R.

Advantages of Rcpp

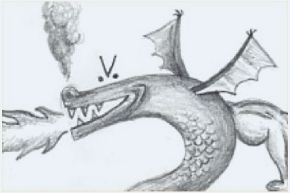
- Compiled code is *fast*.
- Easy to install.
- Easy to use (comparatively).
- Better documented than alternatives.
- Large, friendly, helpful community.

Rcpp Package Dependencies



Disadvantages

- It's C++ (there be dragons).
- Difficult to debug/profile.
- Rcpp designed to only work with R.



7 Introduction to Rcpp
- Foreign Language Interfaces
- What is Rcpp?
- Documentation and Help

Documentation

- The numerous Rcpp vignettes http://cran.r-project.org/web/packages/Rcpp/index.html (start with Introduction, quickref, and FAQ).
- *High Performance Functions with Rcpp*, Hadley Wickham: http://adv-r.had.co.nz/Rcpp.html
- *Seamless R and C++ Integration with Rcpp* (book), http://www.amazon.com/Seamless-Integration-Rcpp-Dirk-Eddelbuettel/dp/1461468671/ref=sr_1_1?ie=UTF8

Where to Get Help

- The documentation.
- The [rcpp] tag on stackoverflow.
- Rcpp-devel list: http://lists.r-forge.r-project.org/mailman/listinfo/rcpp-devel

Advice

New to C++?

- Get a good book on just C++.
- Be patient. C++ is really hard.
- Learn the art of reading template explosions.

Know R?

- Never use `.` in object names.
- Lines end with `;`.
- Returns of functions must be explicitly named.

Know C++?

- No voids.
- If data is modified, do it in a copy.
- R functions are not thread safe!!!

8 Using Rcpp
- C vs Rcpp
- Using Rcpp with R

C/C++ API's and Extensions for R

- The native C interface.
- Rcpp
  - RcppArmadillo
  - RcppCNPy
  - RcppEigen
  - RcppGSL
  - RcppRedis
  - ...
- Rcpp11, Rcpp14, ...

C vs Rcpp

To see the difference, let's construct:

```r
list(a=1L, b=2.0)
```

using the native C interface and with Rcpp.

The C Interface

```c
#include <R.h>
#include <Rinternals.h>

SEXP examplefun(){
  SEXP ret, retnames, a, b;
  PROTECT(a = allocVector(INTSXP, 1));
  PROTECT(b = allocVector(REALSXP, 1));

  INTEGER(a)[0] = 1;
  REAL(b)[0] = 2.0;

  PROTECT(ret = allocVector(VECSXP, 2));
  SET_VECTOR_ELT(ret, 0, a);
  SET_VECTOR_ELT(ret, 1, b);

  PROTECT(retnames = allocVector(STRSXP, 2));
  SET_STRING_ELT(retnames, 0, mkChar("a"));
  SET_STRING_ELT(retnames, 1, mkChar("b"));
  setAttrib(ret, R_NamesSymbol, retnames);

  UNPROTECT(4);
  return ret;
}
```

Rcpp

```
#include <Rcpp.h>

// [[Rcpp::export]]
Rcpp::List examplefun()
{
  Rcpp::IntegerVector a(1);
  Rcpp::NumericVector b(1);

  a[0] = 1;
  b[0] = 2.0;

  Rcpp::List ret =
    Rcpp::List::create(Rcpp::Named("a") = a,
                       Rcpp::Named("b") = b);

  return ret;
}
```

C vs Rcpp

- I can't in good conscience describe C++ as *good for beginners*.
- Rcpp is cleaner.
- Like C++? You'll *love* Rcpp.

8 Using Rcpp
- C vs Rcpp
- Using Rcpp with R

Rcpp

What about compiling, linking, loading, wrapping, etc?

Building with Rcpp

We will be using `sourceCpp()` to build our examples:

1. Create C++ function as string in R.
2. Use sourceCpp to generate wrapper.
3. Call your function in R.

sourceCpp(): Create C++ Function

```
code <- '
#include <Rcpp.h>

// [[Rcpp::export]]
int plustwo(int n)
{
  return n+2;
}
'
```

sourceCpp(): Use sourceCpp

```r
library(Rcpp)
sourceCpp(code=code)
```

sourceCpp(): Call Your Function in R

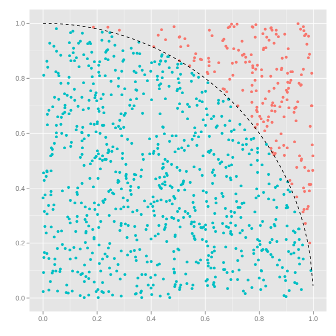
```r
plustwo(1)
# [1] 3
```

9 The Typical Monte Carlo Simulation for Estimating π

Example 1 : Monte Carlo Simulation to Extimate π

Sample N uniform observations (x_i, y_i) in the unit square $[0,1] \times [0,1]$. Then

$$\pi \approx 4\left(\frac{\#\ Inside\ Circle}{\#\ Total}\right) = 4\left(\frac{\#\ \text{Blue}}{\#\ \text{Blue} + \#\ \text{Red}}\right)$$



Outline

1. Implement in R using loops.
2. Implement in R using vectorization.
3. Implement in C++ with Rcpp.
4. Benchmark.
5. Examine other performance considerations.

9 The Typical Monte Carlo Simulation for Estimating π

- Background and Outline
- Implementation
- Summary

Example 1: Monte Carlo Simulation Code

R Code (loops)

```
mcsim_r <- function(n)
{
  r <- 0L

  for (i in 1:n){
    u <- runif(1)
    v <- runif(1)

    if (u^2 + v^2 <= 1)
      r <- r + 1
  }

  return( 4*r/n )
}
```

Example 1: Monte Carlo Simulation Code

R Code (vectorized)

```
mcsim_r_vec <- function(n)
{
  x <- matrix(runif(n * 2), ncol=2)
  r <- sum(rowSums(x^2) <= 1)

  return( 4*r/n )
}
```

Example 1: Monte Carlo Simulation Code

Rcpp Code

```
code <- "
#include <Rcpp.h>

// [[Rcpp::export]]
double mcsim_rcpp(const int n)
{
  int i, r = 0;
  double u, v;

  for (i=0; i<n; i++){
    u = R::runif(0, 1);
    v = R::runif(0, 1);

    if (u*u + v*v <= 1)
      r++;
  }

  return (double) 4.*r/n;
}
"

library(Rcpp)
sourceCpp(code=code)
```

Example 1: Monte Carlo Simulation Code

Benchmarking the Methods

```r
library(rbenchmark)

n <- 100000L

benchmark(R.loop = mcsim_r(n),
          R.vec = mcsim_r_vec(n),
          C = mcsim_c(n),
          Rcpp = mcsim_rcpp(n),
          columns=c("test", "replications", "elapsed",
              "relative"))
```

```
    test replications elapsed relative
3   Rcpp          100   0.309    1.000
1 R.loop          100  65.543  212.113
2  R.vec          100   1.989    6.437
```

Example 1: Monte Carlo Simulation Code

Benchmarking the Methods

```r
library(rbenchmark)

n <- 10000000L

benchmark(R.vec = mcsim_r_vec(n),
          Rcpp = mcsim_rcpp(n),
          columns=c("test", "replications", "elapsed",
              "relative"))
```

```
    test replications elapsed relative
2   Rcpp          100  30.825    1.000
1  R.vec          100 135.075    4.382
```

What About the Compiler?

Benchmarking the Methods

```r
library(rbenchmark)
library(compiler)

mcsim_r <- cmpfun(mcsim_r)
mcsim_r_vec <- cmpfun(mcsim_r_vec)
mcsim_rcpp <- cmpfun(mcsim_rcpp)

n <- 100000L

benchmark(R.loop = mcsim_r(n),
          R.vec = mcsim_r_vec(n),
          Rcpp = mcsim_rcpp(n),
          columns=c("test", "replications", "elapsed",
              "relative"))
```

```
    test replications elapsed relative
3   Rcpp          100   0.311    1.000
1 R.loop          100  55.125  177.251
2  R.vec          100   1.107    3.559
```

Memory Usage in Bytes (roughly)

Loops:

$$\underbrace{4(n+3)}_{\text{Integers}} + \underbrace{8 \cdot 3}_{\text{Doubles}}$$

Vectorized:

$$\underbrace{4n}_{\text{Integers}} + \underbrace{8(2+2n)}_{\text{Doubles}}$$

Rcpp

$$\underbrace{4 \cdot 3}_{\text{Integers}} + \underbrace{8 \cdot 3}_{\text{Doubles}}$$

9 The Typical Monte Carlo Simulation for Estimating π

- Background and Outline
- Implementation
- Summary

Summary

For $n = 100,000$ iterations and 100 replicates:

	Loops	Vectorized	Rcpp
Avg Runtime (seconds)	0.65543	0.01999	0.00309
Avg Compiled Runtime (seconds)	0.55125	0.1107	0.00311
Memory Usage	1.526 MiB	13.733 MiB	36 bytes

Processor:	Core i5 Sandy Bridge
R Version:	3.1.2
C++ Compiler:	clang++ 3.5.0
CXX Flags:	`-O3 -fpic`

Some Thoughts

- Bad R often looks like good C/C++.
- The bytecode compiler helps, but not much.
- R's memory footprint is terrible.

10 Computing the Cosine Similarity Matrix

- Background and Outline
- Implementation
- Benchmarks
- Summary

Cosine Similarity

Recall from vector calculus that for vectors x and y

$$cos(x, y) = \|x\| \, \|y\| \, \cos(\theta(x, y))$$

We define

$$\text{cosim}(x, y) := \cos(\theta(x, y)) = \frac{x \cdot y}{\|x\| \, \|y\|}$$

Cosine Similarity Matrix

The cosine similarity matrix of a given (possibly non-square) matrix is the matrix of all pairwise similarities of the columns, i.e., given

$$X_{n,p} = [x_1, \dots, x_p]$$

We take

$$\mathrm{cosim}(X)_{ij} = \mathrm{cosim}(x_i, x_j)$$

10 Computing the Cosine Similarity Matrix

- Background and Outline
- Implementation
- Benchmarks
- Summary

Original implementation

From CRAN's lsa package version 0.73 (in R/lsa.R)

```
cosine <- function (x, y = NULL){
    if (is.matrix(x) && is.null(y)) {
        co = array(0, c(ncol(x), ncol(x)))
        f = colnames(x)
        dimnames(co) = list(f, f)
        for (i in 2:ncol(x)) {
            for (j in 1:(i - 1)) {
                co[i, j] = cosine(x[, i], x[, j])
            }
        }
        co = co + t(co)
        diag(co) = 1
        return(as.matrix(co))
    }
    else if (is.vector(x) && is.vector(y))
        return(crossprod(x, y)/sqrt(crossprod(x) * crossprod(y)))
    else
        stop("argument mismatch.")
}
```

R Improvements 1

```r
cosine_loop <- function(x){
  cp <- crossprod(x)
  dg <- diag(cp)

  co <- matrix(0.0, length(dg), length(dg))

  for (j in 2L:length(dg)){
    for (i in 1L:(j-1L)){
      co[i, j] <- cp[i, j] / sqrt(dg[i] * dg[j])
    }
  }

  co <- co + t(co)
  diag(co) <- 1.0

  return( co )
}
```

Rcpp 1

```
library(Rcpp)

code <- "
#include <Rcpp.h>

// [[Rcpp::export]]
Rcpp::NumericMatrix fill_loop(Rcpp::NumericMatrix cp,
    Rcpp::NumericVector dg){
  const unsigned int n = cp.nrow();
  Rcpp::NumericMatrix co(n, n);

  // Fill lower triangle and diagonal
  for (int j=0; j<n; j++){
    for (int i=0; i<=j; i++){
      if (i == j)
        co(j, j) = 1.0;
      else
        co(i, j) = cp(i, j) / std::sqrt(dg[i] * dg[j]);
    }
  }

```

Rcpp 2

```
  // Copy lower triangle to upper
  for (int j=0; j<n; j++){
    for (int i=j+1; i<n; i++)
      co(i, j) = co(j, i);
  }

  return co;
}
"
sourceCpp(code=code)


cosine_Rcpp <- function(x){
  cp <- crossprod(x)
  dg <- diag(cp)

  co <- fill_loop(cp, dg)

  return( co )
}
```

10 Computing the Cosine Similarity Matrix

- Background and Outline
- Implementation
- Benchmarks
- Summary

Rcpp 1

```
library(rbenchmark)

reps <- 10

for (i in 1:10){
  n <- i*100
  x <- matrix(rnorm(n*n), n, n)

  benchmark(cosine(x), cosine_loop(x), cosine_Rcpp(x), replications=reps, columns=c("test",
"relative"))
}
```

Relative Performance

Matrix Dimension	cosine()	cosine_loop()	cosine_Rcpp()
100x100	340	44.5	1
200x200	535.167	57	1
300x300	441.632	42.895	1
400x400	495.176	42.412	1
500x500	519.877	41.456	1
600x600	512.264	36.758	1
700x700	392.114	25.486	1
800x800	474.341	28.498	1
900x900	523.841	29.367	1
1000x1000	459.322	23.995	1

Relative Performance with Bytecode Compilation

Matrix Dimension	cosine()	cosine_loop()	cosine_Rcpp()
100x100	300	25.5	1
200x200	360.25	25.125	1
300x300	454.059	29.941	1
400x400	252.885	14.705	1
500x500	315.518	17.671	1
600x600	323.662	15.398	1
700x700	430.507	18.169	1
800x800	385.504	15.043	1
900x900	469.728	16.709	1
1000x1000	505.706	16.625	1

10 Computing the Cosine Similarity Matrix

Summary

- Bad R often looks like good C/C++.
- Compiled code can be much faster than R code.
- Vectorized code better than loops, but worse than more tailored compiled code.

Exercises

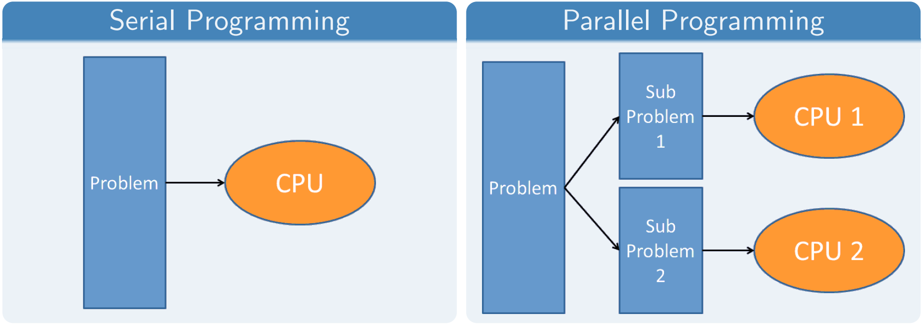
Part IV

Parallelism

11 An Overview of Parallelism

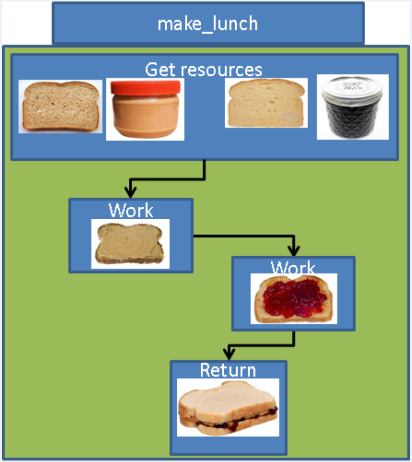
- Terminology: Parallelism
- Guidelines
- Summary

Parallelism

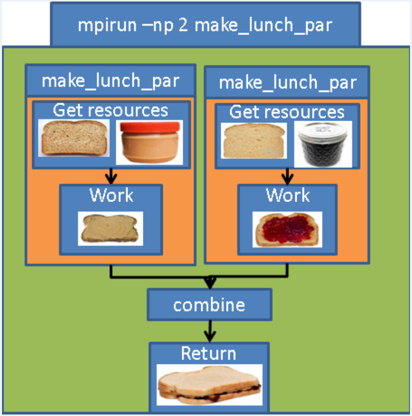


Parallelism

Serial Programming



Parallel Programming



Parallel Programming Vocabulary: Difficulty in Parallelism

1. *Implicit parallelism*: Parallel details hidden from user
   Example: Using multi-threaded BLAS

2. *Explicit parallelism*: Some assembly required...
   Example: Using the `mclapply()` from the **parallel** package

3. *Embarrassingly Parallel* or *loosely coupled*: Obvious how to make parallel; lots of independence in computations.
   Example: Fit two independent models in parallel.

4. *Tightly Coupled*: Opposite of embarrassingly parallel; lots of dependence in computations.
   Example: Speed up model fitting for one model.

Speedup

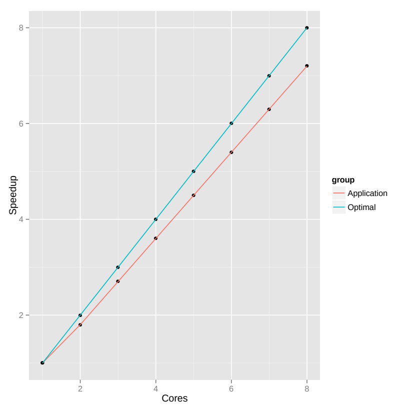
- *Wallclock Time*: Time of the clock on the wall from start to finish
- *Speedup*: unitless measure of improvement; more is better.

$$S_{n_1,n_2} = \frac{\text{Time for } n_1 \text{ cores}}{\text{Time for } n_2 \text{ cores}}$$

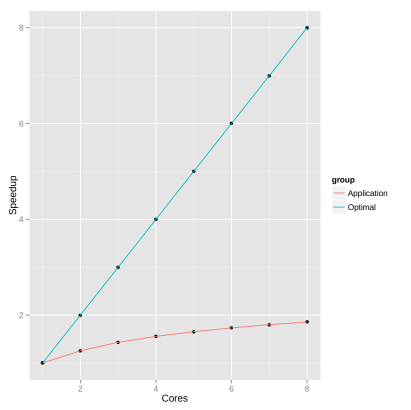
  - n_1 is often taken to be 1
  - In this case, comparing parallel algorithm to serial algorithm

Speedup

Good Speedup



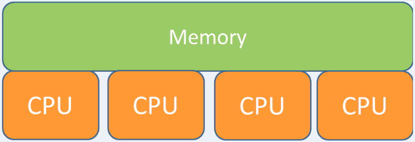
Bad Speedup



Shared and Distributed Memory Machines

Shared Memory

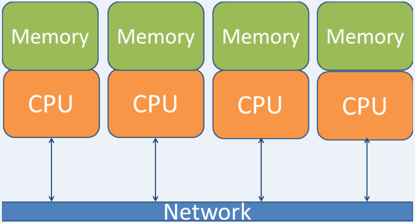
Direct access to read/change memory (one node)



Examples: laptop, GPU, MIC

Distributed

No direct access to read/change memory (many nodes); requires communication



Examples: cluster, server, supercomputer

Shared and Distributed Memory Machines

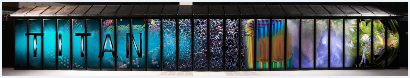
Shared Memory Machines

Thousands of cores

Nautilus, University of Tennessee
1024 cores
4 TB RAM

Distributed Memory Machines

Hundreds of thousands of cores



Titan, Oak Ridge National Lab
299,008 cores
584 TB RAM

Parallel Programming Packages for R

Shared Memory

Examples: **parallel**, **snow**, **foreach**, **gputools**, **HiPLARM**

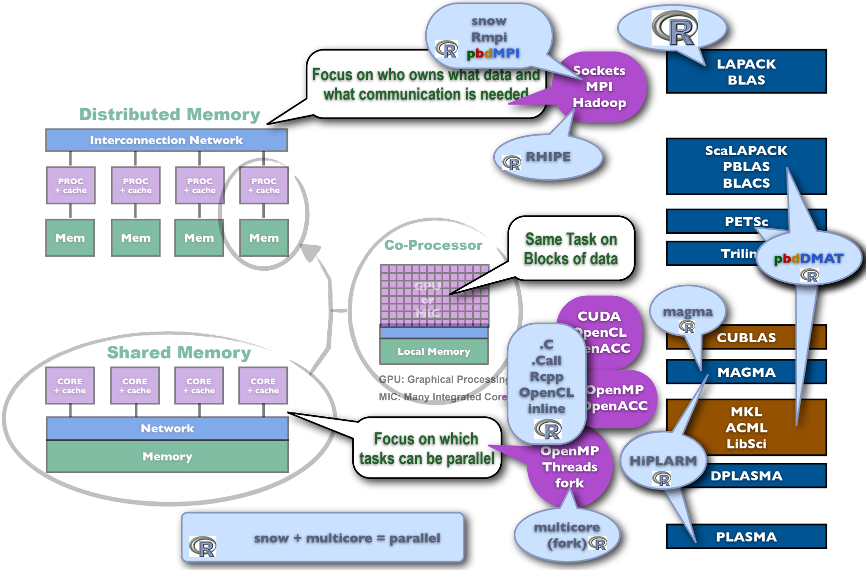
Distributed

Examples: **pbdR**, **Rmpi**, **RHadoop**, **RHIPE**

CRAN HPC Task View

For more examples, see: `http://cran.r-project.org/web/views/HighPerformanceComputing.html`

Parallel Programming Packages for R

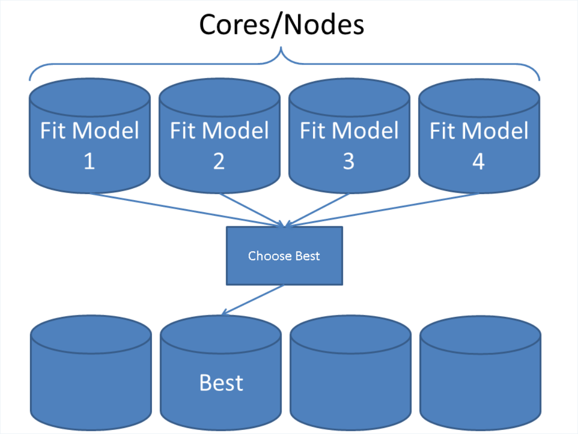


11 An Overview of Parallelism

- Terminology: Parallelism
- Guidelines
- Summary

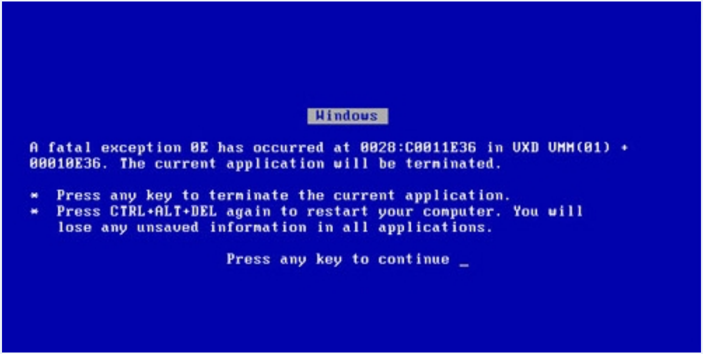
Independence

- Parallelism requires *independence*.
- Separate evaluations of R functions is embarrassingly parallel.



Portability

Many parallel R packages break on Windows



RNG's in Parallel

- Be careful!
- Aided by **rlecuyer**, **rsprng**, and **doRNG** packages.

Parallel Programming: In Theory

Parallel Programming: In Practice

11 An Overview of Parallelism

- Terminology: Parallelism
- Guidelines
- Summary

Summary

- Many kinds of parallelism available to R.
- Better/parallel BLAS is free speedup for linear algebra, but takes some work.

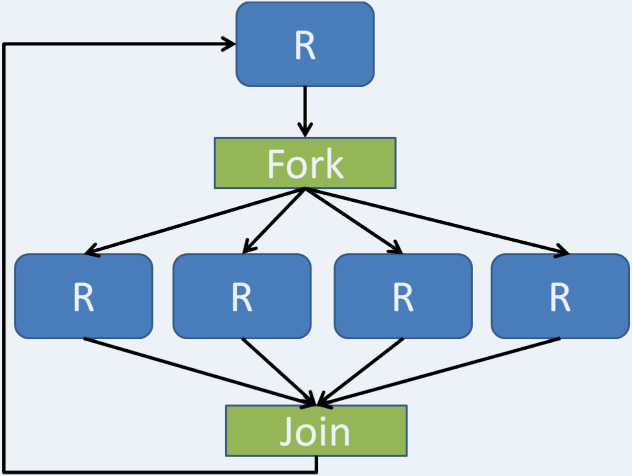
The parallel Package

- Comes with R $\geq$ 2.14.0
- Has 2 disjoint interfaces.

parallel $=$ **snow** $+$ **multicore**

The parallel Package: multicore

Operates on fork/join paradigm.



The parallel Package: multicore

+ Data copied to child on write (handled by OS)
+ Very efficient.
- No Windows support.
- Not as efficient as threads.

The parallel Package: multicore

```r
mclapply(X, FUN, ...,
  mc.preschedule=TRUE, mc.set.seed=TRUE,
  mc.silent=FALSE, mc.cores=getOption("mc.cores", 2L),
  mc.cleanup=TRUE, mc.allow.recursive=TRUE)
```

```r
x <- lapply(1:10, sqrt)

library(parallel)
x.mc <- mclapply(1:10, sqrt)

all.equal(x.mc, x)
# [1] TRUE
```

The parallel Package: multicore

```
simplify2array(mclapply(1:10, function(i) Sys.getpid(),
    mc.cores=4))
# [1] 27452 27453 27454 27455 27452 27453 27454 27455 27452
    27453

simplify2array(mclapply(1:2, function(i) Sys.getpid(),
    mc.cores=4))
# [1] 27457 2745
```

The parallel Package: snow

? Uses sockets.

+ Works on all platforms.

- More fiddley than `mclapply()`.

- Not as efficient as forks.

The parallel Package: snow

```r
### Set up the worker processes
cl <- makeCluster(detectCores())
cl
# socket cluster with 4 nodes on host   localhost

parSapply(cl, 1:5, sqrt)

stopCluster(cl)
```

The parallel Package: Summary

All

- `detectCores()`
- `splitIndices()`

multicore

- `mclapply()`
- `mcmapply()`
- `mcparallel()`
- `mccollect()`
- and others. . .

snow

- `makeCluster()`
- `stopCluster()`
- `parLapply()`
- `parSapply()`
- and others. . .

12 Shared Memory Parallelism in R

- The parallel Package
- The foreach Package

The foreach Package

- On Cran (Revolution Analytics).
- Main package is **foreach**, which is a single interface for a number of "backend" packages.
- Backends: **doMC**, **doMPI**, **doParallel**, **doRedis**, **doRNG**, **doSNOW**.

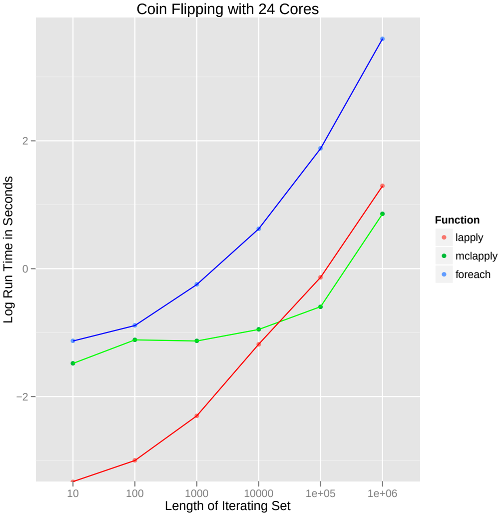
The foreach Package: The Idea

Unify the disparate interfaces.

The foreach Package

- \+ Works on all platforms (if backend does).
- \+ Can even work serial with minor notational change.
- \+ Write the code once, use whichever backend you prefer.
- \- Really bizarre, non-R-ish synatx.
- \- Efficiency issues if you aren't careful!

Efficiency Issues




```r
### Bad performance
foreach(i=1:len) %dopar% tinyfun(i)

### Expected performance
foreach(i=1:ncores) %dopar% {
  out <- numeric(len/ncores)
  for (j in 1:(len/ncores))
    out[i] <- tinyfun(j)
  out
}
```

The foreach Package: General Procedure

- Load **foreach** and your backend package.
- Register your backend.
- Call `foreach`

Using foreach: serial

```r
library(foreach)

### Example 1
foreach(i=1:3) %do% sqrt(i)

### Example 2
n <- 50
reps <- 100

x <- foreach(i=1:reps) %do% {
  sum(rnorm(n, mean=i)) / (n*reps)
}
```

Using foreach: Parallel

```r
library(foreach)
library(<mybackend>)

register<MyBackend>()

### Example 1
foreach(i=1:3) %dopar% sqrt(i)

### Example 2
n <- 50
reps <- 100

x <- foreach(i=1:reps) %dopar% {
  sum(rnorm(n, mean=i)) / (n*reps)
}
```

foreach backends

multicore

```r
library(doParallel)
registerDoParallel(cores=ncores)
foreach(i=1:2) %dopar% Sys.getpid()
```

snow

```r
library(doParallel)
cl <- makeCluster(ncores)
registerDoParallel(cl=cl)

foreach(i=1:2) %dopar% Sys.getpid()
stopCluster(cl)
```

foreach Summary

- Make sure to register your backend.
- Different backends may have different performance.
- Use `%dopar%` for parallel foreach.
- `%do%` and `%dopar%` *must* appear on the same line as the `foreach()` call.

Why Distribute?

- Nodes only hold so much ram.
- Commodity hardware: $\approx 32 - 64$ gib.
- With a few exceptions (**ff**, **bigmemory**), R does computations in memory.
- If your problem doesn't fit in the memory of one node...

Packages for Distributed Memory Parallelism in R

- **Rmpi**, and **snow** via **Rmpi**.
- **RHIPE** and **RHadoop** ecosystem.
- **pbdR** ecosystem.

Hasty Explanation of MPI

- MPI = Message Passing Interface
- Recall: Distributed machines can't directly manipulate memory of other nodes.
- Can *indirectly* manipulate them, however...
- Distinct nodes collaborate by passing messages over network.

13 Distributed Memory Parallelism with R

Rmpi Hello World

```
mpi.spawn.Rslaves(nslaves=2)
#          2 slaves are spawned successfully. 0 failed.
# master (rank 0, comm 1) of size 3 is running on: wootabega
# slave1 (rank 1, comm 1) of size 3 is running on: wootabega
# slave2 (rank 2, comm 1) of size 3 is running on: wootabega

mpi.remote.exec(paste("I
    am",mpi.comm.rank(),"of",mpi.comm.size()))
# $slave1
# [1] "I am 1 of 3"
#
# $slave2
# [1] "I am 2 of 3"

mpi.exit()
```

Using Rmpi from snow

```
library(snow)
library(Rmpi)

cl <- makeCluster(2, type = "MPI")
clusterCall(cl, function() Sys.getpid())
clusterCall(cl, runif, 2)
stopCluster(cl)
mpi.quit()
```

Rmpi Resources

- **Rmpi** tutorial: `http://math.acadiau.ca/ACMMaC/Rmpi/`
- **Rmpi** manual: `http://cran.r-project.org/web/packages/Rmpi/Rmpi.pdf`

13 Distributed Memory Parallelism with R

- Distributed Memory Parallelism
- Rmpi
- pbdMPI vs Rmpi
- Summary

pbdMPI vs Rmpi

- **Rmpi** is interactive; **pbdMPI** is exclusively batch.
- **pbdMPI** is easier to install.
- **pbdMPI** has a simpler interface.
- **pbdMPI** integrates with other pbdR packages.

Example Syntax

Rmpi

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

pbdMPI

```
allreduce(x)
```

Types in R

```
> typeof(1)
[1] "double"
> typeof(2)
[1] "double"
> typeof(1:2)
[1] "integer"
```

13 Distributed Memory Parallelism with R

- Distributed Memory Parallelism
- Rmpi
- pbdMPI vs Rmpi
- **Summary**

Summary

- Distributed parallelism is necessary when computations no longer fit in ram.
- Several options available; most go beyond the scope of this talk.

Recall: Parallel R Packages

Shared Memory

1. **foreach**
2. **parallel**
3. **snow**
4. **multicore**

Distributed

1. **Rmpi**
2. **RHIPE, RHadoop**
3. **pbdR**

(and others...)

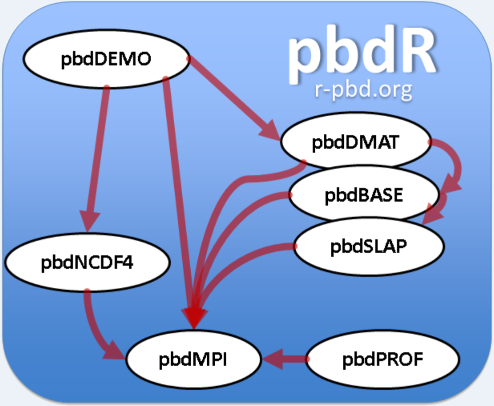
Programming with Big Data in R (pbdR)

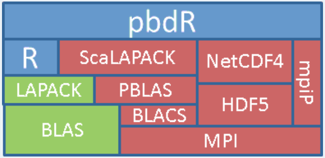
Striving for *Productivity, Portability, Performance*

- *Free*[a] R packages.
- Bridging high-performance compiled code with high-productivity of R
- Scalable, big data analytics.
- Offers implicit and explicit parallelism.
- Methods have syntax *identical* to R.

[a] MPL, BSD, and GPL licensed

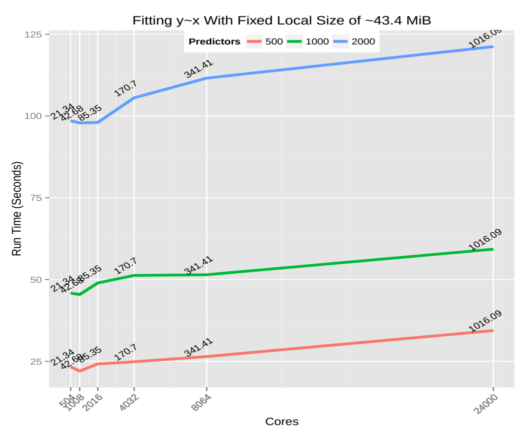
pbdR Packages





Distributed Matrices and Statistics with **pbdDMAT**

Least Squares Benchmark




```r
x <- ddmatrix("rnorm", nrow=m, ncol=n)
y <- ddmatrix("rnorm", nrow=m, ncol=1)
mdl <- lm.fit(x=x, y=y)
```

pbdR Scripts

- They're just R scripts.
- Can't run interactively (with more than 1 rank).
- We can use **pbdinline** to get "pretend interactivity".

ddmatrix: 2-dimensional Block-Cyclic with 6 Processors

$$x = \left[\begin{array}{cc|cc|cc|cc|c} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \left|\begin{array}{ccc} 0 & 1 & 2 \\ 3 & 4 & 5 \end{array}\right| = \left|\begin{array}{ccc} (0,0) & (0,1) & (0,2) \\ (1,0) & (1,1) & (1,2) \end{array}\right|$$

Understanding `ddmatrix`: Local View

$$
\left[\begin{array}{cc|cc}
x_{11} & x_{12} & x_{17} & x_{18} \\
x_{21} & x_{22} & x_{27} & x_{28} \\ \hline
x_{51} & x_{52} & x_{57} & x_{58} \\
x_{61} & x_{62} & x_{67} & x_{68} \\ \hline
x_{91} & x_{92} & x_{97} & x_{98}
\end{array}\right]_{5\times 4}
\quad
\left[\begin{array}{cc|c}
x_{13} & x_{14} & x_{19} \\
x_{23} & x_{24} & x_{29} \\ \hline
x_{53} & x_{54} & x_{59} \\
x_{63} & x_{64} & x_{69} \\ \hline
x_{93} & x_{94} & x_{99}
\end{array}\right]_{5\times 3}
\quad
\left[\begin{array}{cc}
x_{15} & x_{16} \\
x_{25} & x_{26} \\ \hline
x_{55} & x_{56} \\
x_{65} & x_{66} \\ \hline
x_{95} & x_{96}
\end{array}\right]_{5\times 2}
$$

$$
\left[\begin{array}{cc|cc}
x_{31} & x_{32} & x_{37} & x_{38} \\
x_{41} & x_{42} & x_{47} & x_{48} \\ \hline
x_{71} & x_{72} & x_{77} & x_{78} \\
x_{81} & x_{82} & x_{87} & x_{88}
\end{array}\right]_{4\times 4}
\quad
\left[\begin{array}{cc|c}
x_{33} & x_{34} & x_{39} \\
x_{43} & x_{44} & x_{49} \\ \hline
x_{73} & x_{74} & x_{79} \\
x_{83} & x_{84} & x_{89}
\end{array}\right]_{4\times 3}
\quad
\left[\begin{array}{cc}
x_{35} & x_{36} \\
x_{45} & x_{46} \\ \hline
x_{75} & x_{76} \\
x_{85} & x_{86}
\end{array}\right]_{4\times 2}
$$

$$
\text{Processor grid} = \left|\begin{array}{ccc} 0 & 1 & 2 \\ 3 & 4 & 5 \end{array}\right| = \left|\begin{array}{ccc} (0,0) & (0,1) & (0,2) \\ (1,0) & (1,1) & (1,2) \end{array}\right|
$$

Methods for class `ddmatrix`

pbdDMAT has over 100 methods with *identical* syntax to R:

- `` `[` ``, `rbind()`, `cbind()`, ...
- `lm.fit()`, `prcomp()`, `cov()`, ...
- `` `%*%` ``, `solve()`, `svd()`, `norm()`, ...
- `median()`, `mean()`, `rowSums()`, ...

Serial Code

```
cov(x)
```

Parallel Code

```
cov(x)
```

ddmatrix Syntax

```
cov.x <- cov(x)
pca <- prcomp(x)
x <- x[, -1]
col.sd <- apply(x, MARGIN=2, FUN=sd)
```

Part V

Wrapup

16 Wrapup

Performance-Centered Development Model

1. Just get it working.
2. Profile vigorously.
3. Weigh your options.
   - Improve R code? (`lapply()`, vectorization, a package, ...)
   - Incorporate C/C++?
   - Go parallel?
   - Some combination of these...
4. Don't forget the free stuff (BLAS, bytecode compiler, ...).
5. Repeat 2 — 4 until performance is acceptable.

Thanks so much for attending!

Questions?

Followup session: Friday, March 6 from 1:00pm-3:00pm Eastern Time

Please go to `www.xsede.org` and create account if you don't have one already.

Register for training at: `https://portal.xsede.org/course-calendar/-/training-user/class/375/session/618`

Password is: hpcR.