Introduction to High-Performance Computing with R

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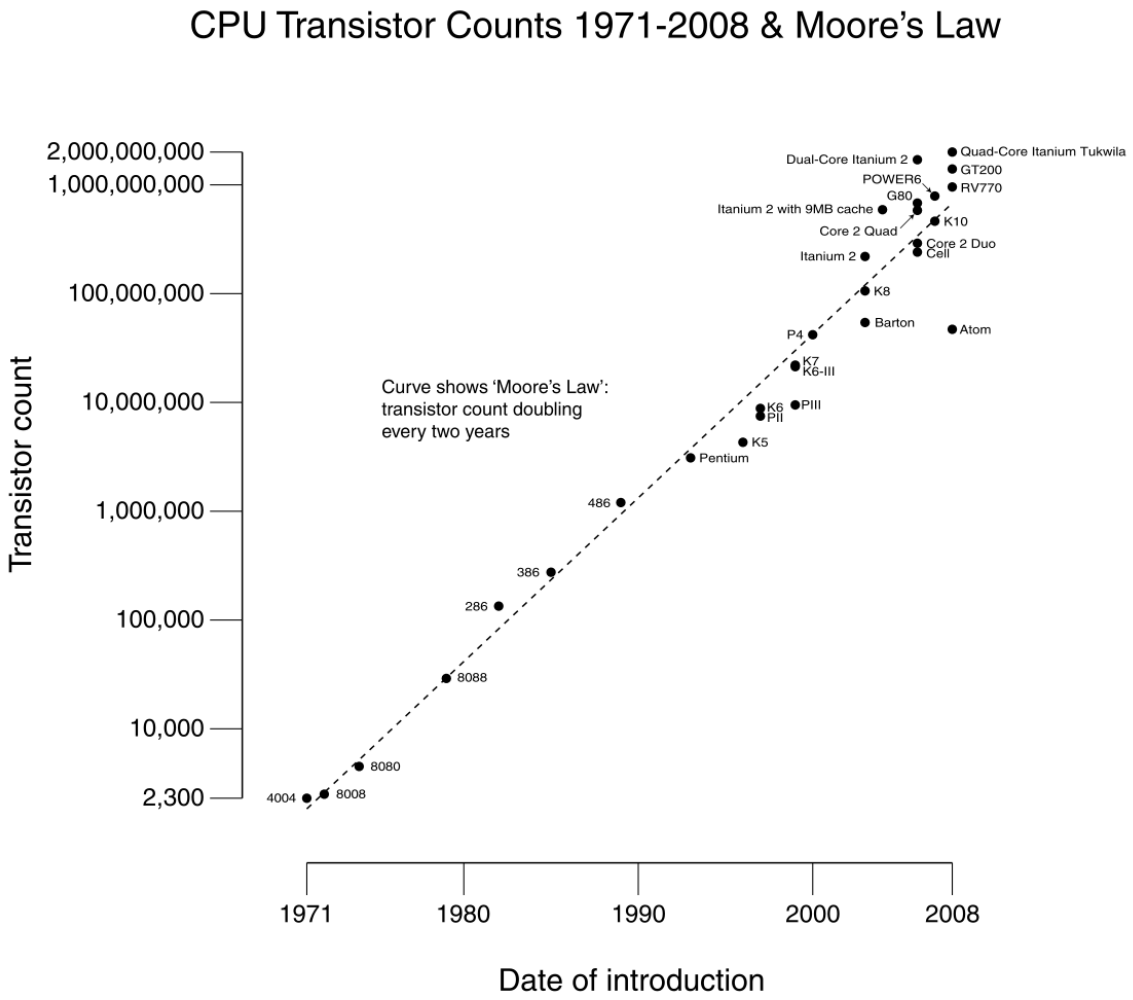
27 November 2009

Outline

Motivation: What describes our current situation?



Source: http://en.wikipedia.org/wiki/Moore's_law

Moore's Law: Processors keep getting *faster and faster*

Yet our datasets get *bigger and bigger* and an even faster rate.

So we're still *waiting and waiting . . .*

Result: An urgent need for *high(er) performance computing* with R.

Motivation: Data sets keep growing

There are a number of reasons behind 'big data':

- *more collection*: everything from faster DNA sequencing to larger experiments to per-item RFID scanning in retail — our ability to *originate* data keeps increasing
- *more networking*: (internet) capacity, transmission speeds and usage keep growing leading to easier ways to assemble data sets from different sources
- *more storage* as what used to be disk capacity is now provided by usb keychains, while data warehousing / data marts are aiming beyond petabytes

Not all large data sets are suitable for R, and data is frequently pruned, filtered or condensed down to *manageable* size (where the exact meaning of manageable will vary by user).

Motivation: Presentation Roadmap

We look at ways to *'script'* running R code which is helpful for both automation and debugging.

We will then *measure* using profiling tools to analyse and visualize performance; we will also look at debugging tools and tricks.

We will look at *vectorisation*, a key method for speed as well as various ways to *compile and use code* before a brief discussion and example of GPU computing.

Next, we will discuss several ways to get more things done at the same time by using simple *parallel computing* approaches.

We will then look at computations *beyond the memory limits*.

A discussion and question sesssion finishes.

Typographics conventions

R itself is highlighted, packages like `Rmpi` get a different color.

External links to e.g. Wikipedia are clickable in the pdf file.

R input and output in different colors, and usually set flush-left so that can show long lines:

```
cat("Hello\n")
```

```
Hello
```

Source code listings are boxed and with lines numbers

```
1 cubed <- function(n) {
2   m <- n^3
3   return(m)
4 }
```

Outline

Tools: Using R in batch mode

Non-interactive use of R is possible:

- Using R in batch mode:

```
$ R --slave < cmdfile.R
$ cat cmdfile.R | R --slave
$ R CMD BATCH cmdfile.R
```

- Using R in here documents is awkward:

```
#!/bin/sh
cat << EOF | R --slave
   a <- 1.23; b <- 4.56
   cat("a times b is", a*b, "\n")
EOF
```

However, this feels somewhat cumbersome. Variable expansion by the shell may interfere as well.

Tools: littler

The `r` frontend provided by the littler package was released by Horner and Eddelbuettel in September 2006 based on Horner's work on rapache.

- execute scripts:
  ```
  $ r somefile.R
  ```
- run Unix pipelines:
  ```
  $ echo 'cat(pi^2, "\n")' | r
  ```
- use arguments:
  ```
  $ r -lboot -e'example(boot.ci)'
  ```
- write Shebang scripts such as `install.r` (see next slide)

littler 'Shebang' example

Consider the following code from the `littler` examples directory:

```
#!/usr/bin/env r
# a simple example to install one or more packages
if (is.null(argv) | length(argv)<1) {
  cat("Usage: installr.r pkg1 [pkg2 pkg3 ...]\n")
  q()
}
## adjust as necessary, see help('download.packages')
repos <- "http://cran.us.r-project.org"
lib.loc <- "/usr/local/lib/R/site-library"
install.packages(argv, lib.loc, repos)
```

Tools: littler cont.

If saved as `install.r`, we can call it via

```
$ install.r ff bigmemory
```

The `getopt` and `optparse` package make it easy for `r` and `Rscript` to support command-line options.

For debugging, the following proves useful:

```
r --package pkgA,pkgB --eval "code(1,2)"
```

We will use a combination of these commands throughout the tutorial.

Tools: littler cont.

A simple example about using pipes:

```
$ du -csk /usr/local/lib/R/site-library/* | \
    awk '!/total$/ {print $1}' | \
    ~/svn/littler/examples/fsizes.r
```

```
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
      4     218     540     864     972    3620

  The decimal point is 3 digit(s) to the right of the |

  0 | 0112335689
  1 | 079
  2 |
  3 | 6
```

This shows that I have a number of small packages installed, as well as one larger one.

Tools: Rscript

`Rscript`, which was first released with R 2.5.0, can be used in a similar fashion.

Due to implementation details, `r` starts up faster than `Rscript`.

On the other hand, `Rscript` is also available on Windows whereas `r` is limited to Linux and OS X.

By providing `r` and `Rscript`, we can now write 'R scripts' that are executable. This allows for automation in cron jobs, Makefile, job queues, ...

RPy

The `RPy` and `RPy2` packages provides access from `Python`:

```
1  from rpy import *
2  set_default_mode(NO_CONVERSION)  # avoid automatic conversion
3  r.library("nnet")
4  model = r("Fxy~x+y")
5  df = r.data_frame(x = r.c(0,2,5,10,15)
6                    ,y = r.c(0,2,5,8,10)
7                    ,Fxy = r.c(0,2,5,8,10))
8  NNModel = r.nnet(model, data = df
9                    , size =10, decay =1e-3
10                   , lineout=True, skip=True
11                   , maxit=1000, Hess =True)
12 XG = r.expand_grid(x = r.seq(0,7,1), y = r.seq(0,7,1))
13 x = r.seq(0,7,1)
14 y = r.seq(0,7,1)
15
16 set_default_mode(BASIC_CONVERSION) # automatic conv. back on
17 fit = r.predict(NNModel,XG)
18 print fit
```

Outline

Profiling

We need to know where our code spends the time it takes to compute our tasks.

Measuring—using *profiling tools*—is critical.

R already provides the basic tools for performance analysis.

- the `system.time` function for simple measurements.
- the `Rprof` function for profiling R code.
- the `Rprofmem` function for profiling R memory usage.

In addition, the `profr` and `proftools` package on CRAN can be used to visualize `Rprof` data.

We will also look at a script from the R Wiki for additional visualization.

Profiling cont.

The chapter *Tidying and profiling R code* in the *R Extensions* manual is a good first source for documentation on profiling and debugging.

Simon Urbanek has a page on benchmarks (for Macs) at `http://r.research.att.com/benchmarks/`

One can also profile compiled code, either directly (using the `gcc` option `-pg`) or by using *e.g.* the Google `perftools` library.

RProf example

Consider the problem of repeatedly estimating a linear model, *e.g.* in the context of Monte Carlo simulation.

The `lm()` workhorse function is a natural first choice.

However, its generic nature as well the rich set of return arguments come at a cost. For experienced users, `lm.fit()` provides a more efficient alternative.

But how much more efficient?

We will use both functions on the `longley` data set.

RProf example cont.

This code runs both approaches 2000 times:

```
data(longley)

# using lm()
Rprof("longley.lm.out")
invisible(replicate(2000,
                    lm(Employed ~ ., data=longley)))
Rprof(NULL)

# using lm.fit()
longleydm <- data.matrix(data.frame(intcp=1, longley))
Rprof("longley.lm.fit.out")
invisible(replicate(2000,
                    lm.fit(longleydm[,-8],    # X
                           longleydm[,8])))   # y
Rprof(NULL)
```

RProf example cont.

We can analyse the output two different ways. First, directly from R into an R object:

```
data <- summaryRprof("longley.lm.out")
print(str(data))
```

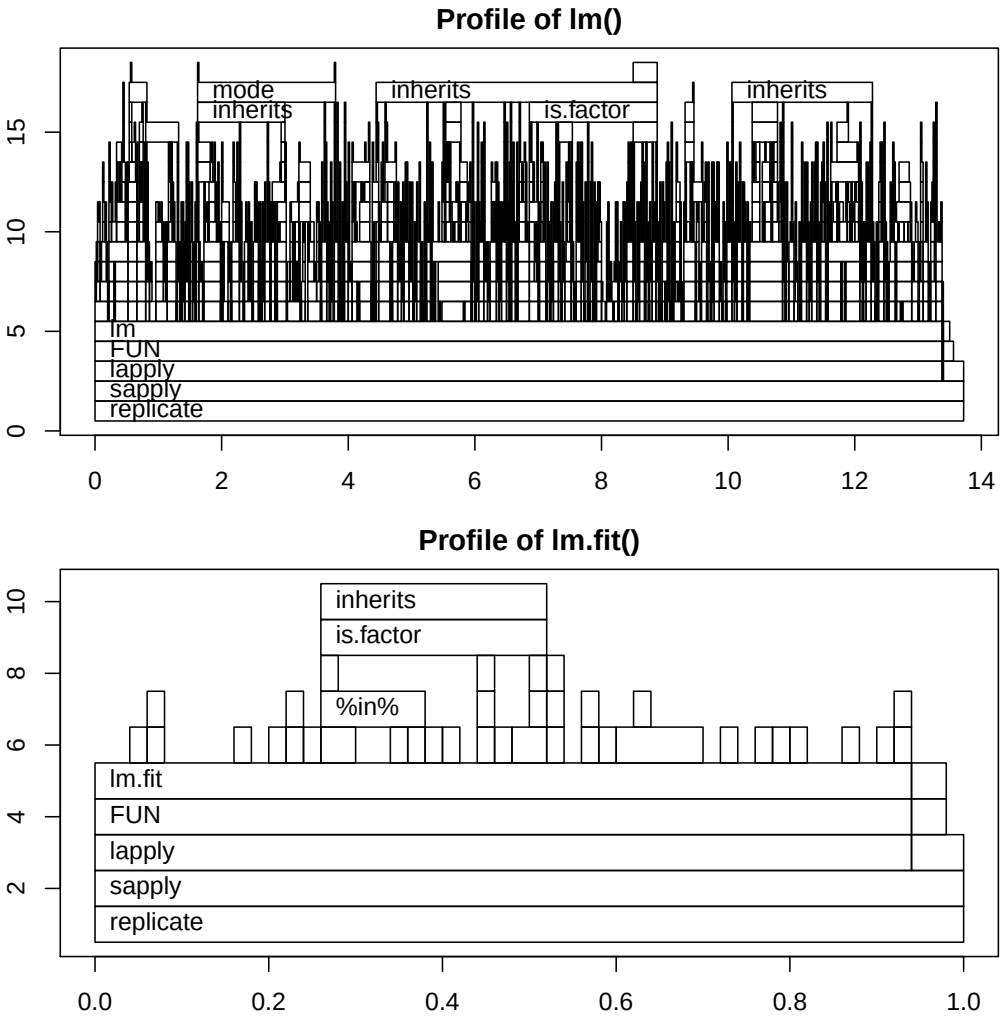
Second, from the command-line (on systems having `Perl`)

```
R CMD Rprof longley.lm.out | less
```

The CRAN package / function `profr` by Hadley Wickham can profile, evaluate, and optionally plot, an expression directly. Or we can use `parse_profr()` to read the previously recorded output:

```
plot(parse_rprof("longley.lm.out"),
                 main="Profile of lm()")
plot(parse_rprof("longley.lm.fit.out"),
                 main="Profile of lm.fit()")
```

RProf example cont.



Source: Our calculations.

Notice the different *x* and *y* axis scales

For the same number of runs, `lm.fit()` is about fourteen times faster as it makes fewer calls to other functions.

RProf example cont.

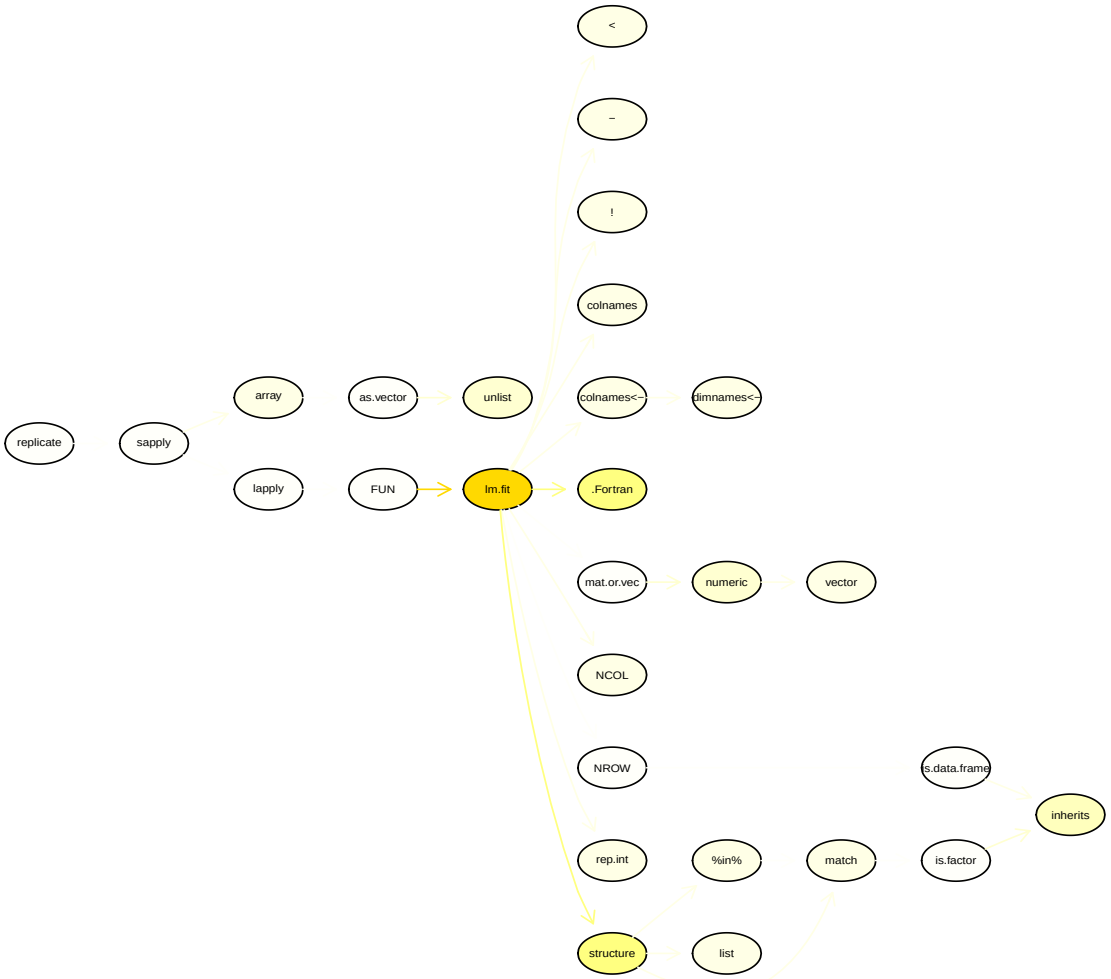
In addition, the `proftools` package by L. Tierney can read profiling data and summarize directly in R.

The `flatProfile` function aggregates the data, optionally with totals.

```
lmfitprod <- readProfileData("longley.lm.fit.out"))
plotProfileCallGraph(lmfitprof)
```

And `plotProfileCallGraph()` can be used to visualize profiling information using the `Rgraphviz` package (which is no longer on CRAN).

RProf example cont.



Color is used to indicate which nodes use the most of amount of time.

Use of color and other aspects can be configured.

Another profiling example

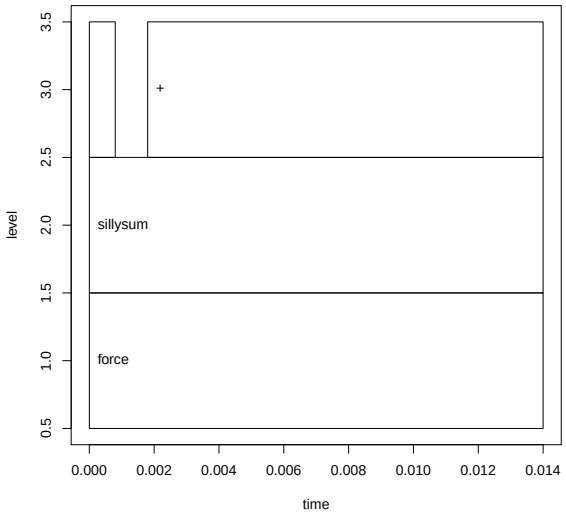
Both packages can be very useful for their quick visualisation of the `RProf` output. Consider this contrived example:

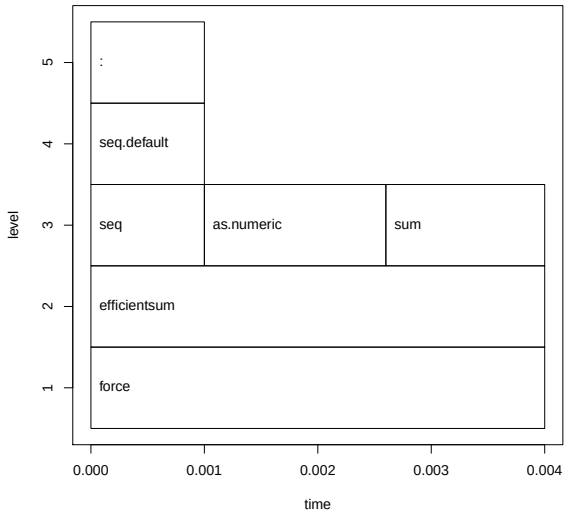
```
sillysum <- function(N) {s <- 0;
      for (i in 1:N) s <- s + i; s}
ival <- 1/5000
plot(profr(a <- sillysum(1e6), ival))
```

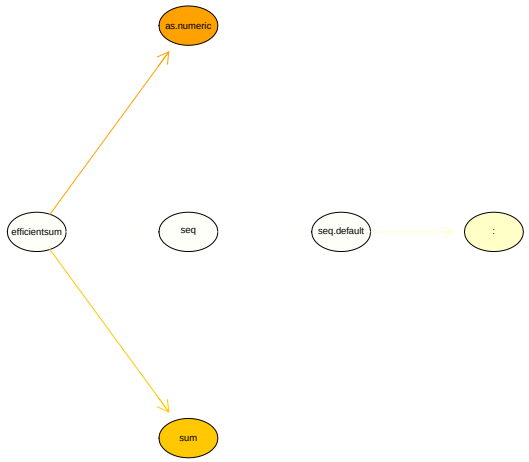
and for a more efficient solution where we use a larger *N*:

```
efficientsum <- function(N) {
sum(as.numeric(seq(1,N))) }
ival <- 1/5000
plot(profr(a <- efficientsum(1e7), ival))
```

Another profiling example (cont.)







`profr` and `proftools` complement each other.

Numerical values in `profr` provide information too.

Choice of colour is useful in `proftools`.

Additional profiling visualizations

Romain Francois has contributed a `Perl` script[1] which can be used to visualize profiling output via the `dot` program (part of `graphviz`):

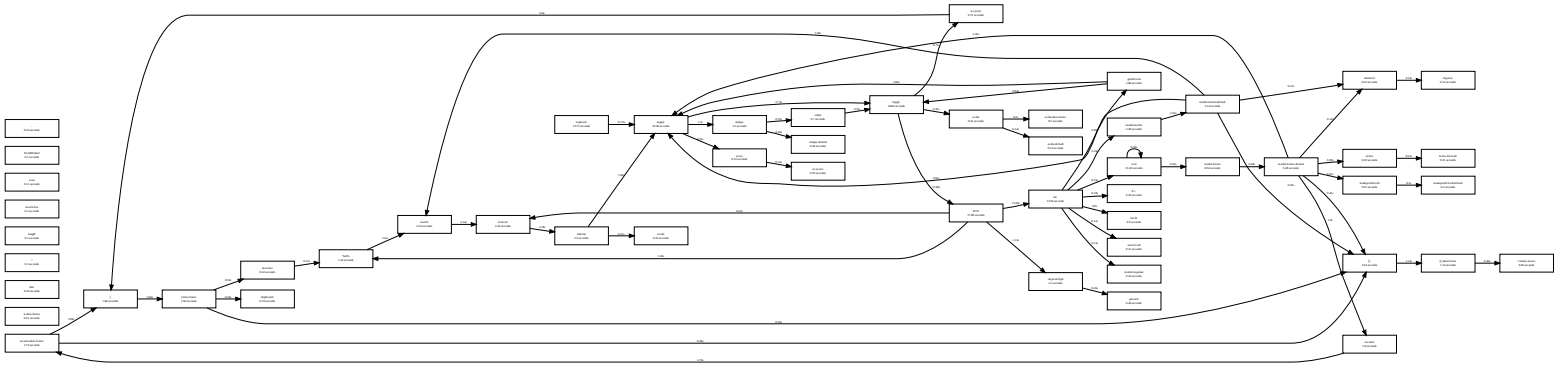
```
./prof2dot.pl longley.lm.out | dot -Tpdf \
              > longley_lm.pdf
./prof2dot.pl longley.lm.fit.out | dot -Tpdf \
              > longley_lmfit.pdf
```

Its key advantages are the ability to include, exclude or restrict functions.

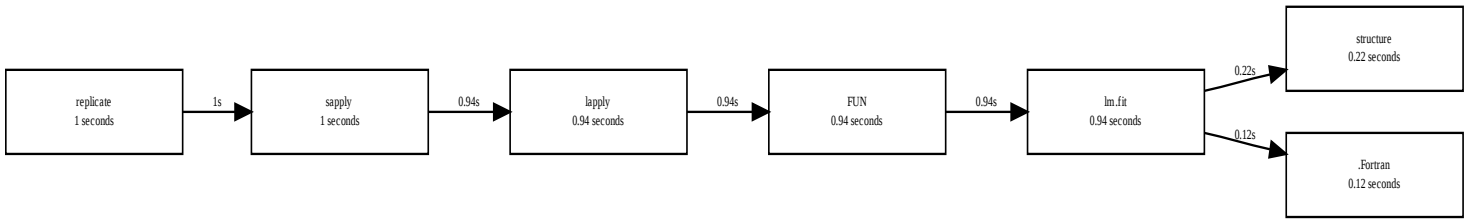
[1] `http://wiki.r-project.org/rwiki/doku.php?id=tips:misc:profiling:current`

Additional profiling visualizations (cont.)

For `lm()`, this yields:



and for `lm.fit()`, this yields:



RProfmem

When R has been built with the `enable-memory-profiling` option, we can also look at use of memory and allocation.

To continue with the *R Extensions* manual example, we issue calls to `Rprofmem` to start and stop logging to a file as we did for `Rprof`. This can be a helpful check for code that is suspected to have an error in its memory allocations.

We also mention in passing that the `tracemem` function can log when copies of a (presumably large) object are being made. Details are in section 3.3.3 of the *R Extensions* manual.

Profiling compiled code

Profiling compiled code typically entails rebuilding the binary and libraries with the `-pg` compiler option. In the case of R, a complete rebuild is required as R itself needs to be compiled with profiling options.

Add-on tools like `valgrind` and `kcachegrind` can be very helpful and may not require rebuilds.

Two other options for Linux are mentioned in the *R Extensions* manual. First, `sprof`, part of the C library, can profile shared libraries. Second, the add-on package `oprofile` provides a daemon that has to be started (stopped) when profiling data collection is to start (end).

A third possibility is the use of the Google Perftools which we will illustrate.

Profiling with Google Perftools

The Google Perftools provide four modes of performance analysis / improvement:

- a thread-caching malloc (memory allocator),
- a heap-checking facility,
- a heap-profiling facility and
- cpu profiling.

Here, we will focus on the last feature.

There are two possible modes of running code with the cpu profiler.

The preferred approach is to link with `-lprofiler`. Alternatively, one can dynamically pre-load the profiler library.

Profiling with Google Perftools (cont.)

```
# turn on profiling and provide a profile log file
LD_PRELOAD="/usr/lib/libprofiler.so.0" \
CPUPROFILE=/tmp/rprof.log \
r profilingSmall.R
```

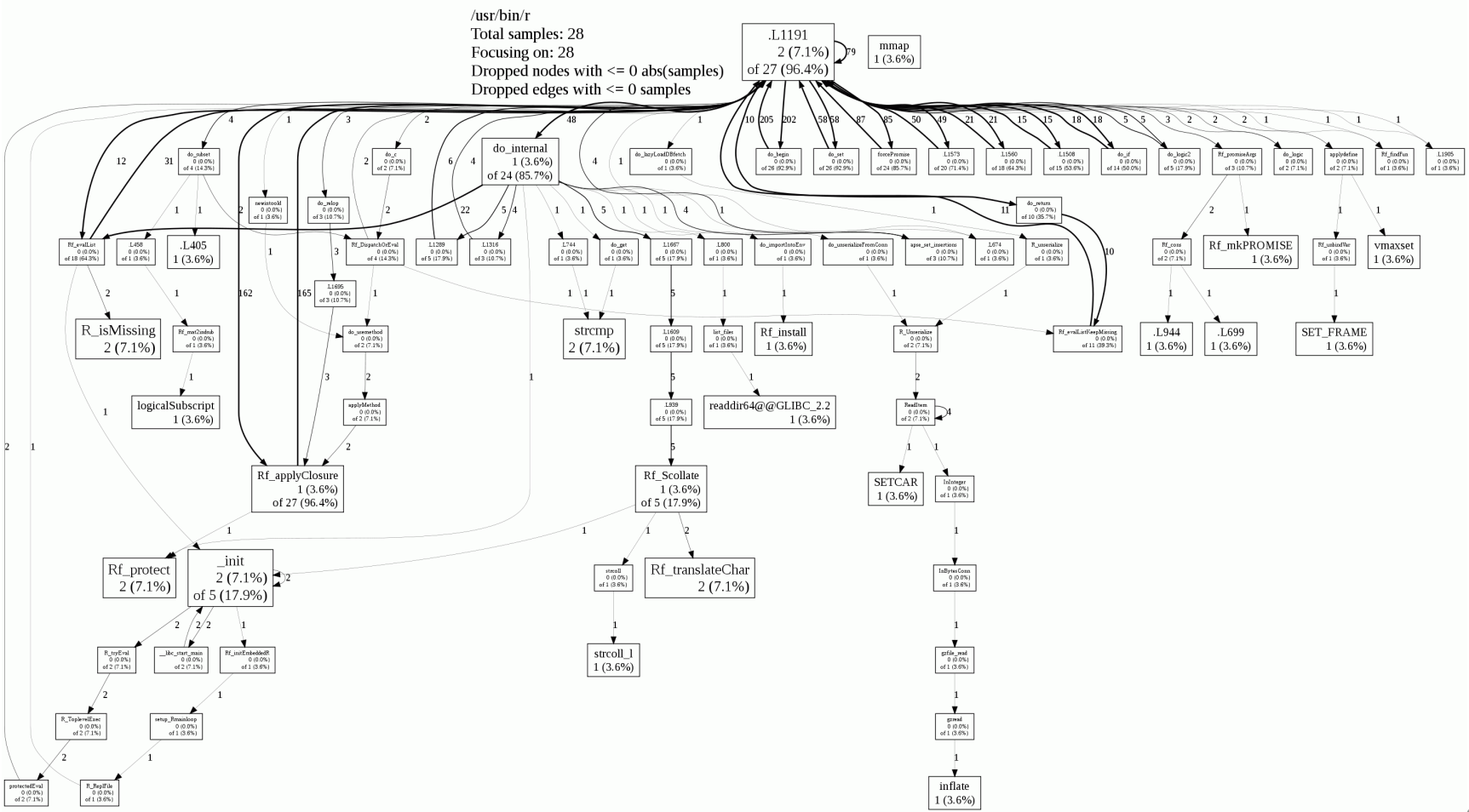
We can then analyse the profiling output in the file. The profiler (renamed from `pprof` to `google-pprof` on Debian) has a large number of options. Here just use two different formats:

```
# show text output
google-pprof --cum --text \
   /usr/bin/r /tmp/rprof.log | less

# or analyse call graph using gv
google-pprof --gv /usr/bin/r /tmp/rprof.log
```

The shell script `googlePerftools.sh` runs the complete example.

Profiling with Google Perftools

This can generate complete (yet complex) graphs.



Profiling with Google Perftools

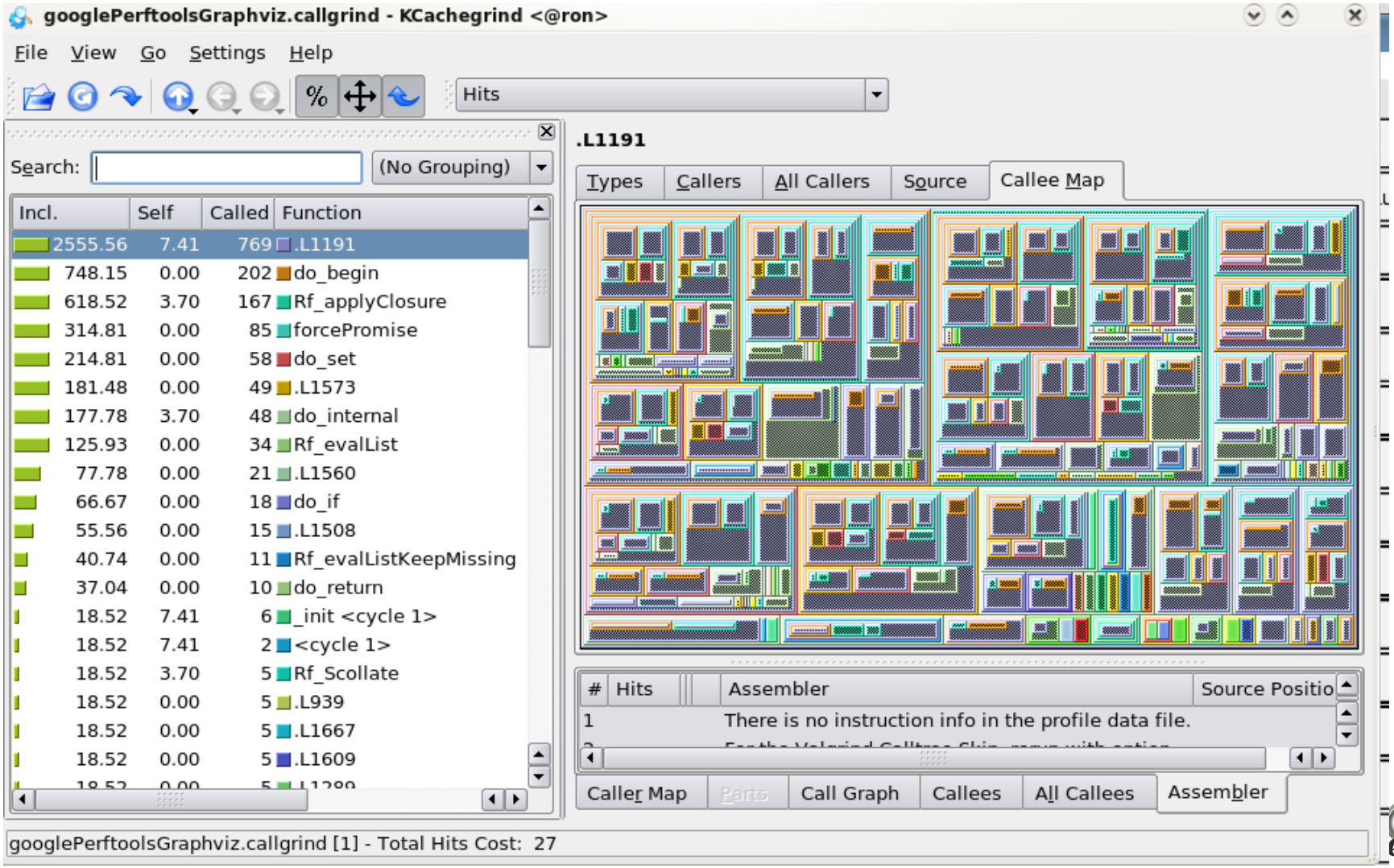
Another output format is used by the *callgrind* analyser that is part of *valgrind*—a frontend to a variety of analysis tools such as *cachegrind* (cache simulator), *callgrind* (call graph tracer), *helpgrind* (race condition analyser), *massif* (heap profiler), and *memcheck* (fine-grained memory checker).

For example, the KDE frontend *kcachegrind* can be used to visualize the profiler output as follows:

```
google-pprof --callgrind \
   /usr/bin/r /tmp/gpProfile.log \
   > googlePerftools.callgrind
kcachegrind googlePerftools.callgrind
```

Profiling with Google Perftools

Kcachegrind running on the the profiling output looks as follows:



Profiling with Google Perftools

One problem with the 'global' approach to profiling is that a large number of internal functions are being reported as well—this may obscure our functions of interest.
An alternative is to re-compile the portion of code that we want to profile, and to bracket the code with

```
ProfilerStart()

// ... code to be profiled here ...

ProfilerEnd()
```

which are defined in `google/profiler.h` which needs to be included. One uses the environment variable `CPUPROFILE` to designate an output file for the profiling information, or designates a file as argument to `ProfilerStart()`.

Outline

Vectorisation

Revisiting our trivial trivial example from the preceding section:

```
> sillysum <- function(N) { s <- 0;
      for (i in 1:N) s <- s + i; return(s) }
> system.time(print(sillysum(1e7)))

[1] 5e+13
   user  system elapsed
 13.617   0.020  13.701
>

> system.time(print(sum(as.numeric(seq(1,1e7)))))

[1] 5e+13
   user  system elapsed
  0.224   0.092   0.315
>
```

Replacing the loop yielded a gain of a factor of more than 40. It really pays to know the corpus of available functions.

Vectorisation cont.

A more interesting example is provided in a case study on the `Ra` (c.f. next section) site and taken from the *S Programming* book:

> *Consider the problem of finding the distribution of the determinant of a 2 x 2 matrix where the entries are independent and uniformly distributed digits 0, 1, . . ., 9. This amounts to finding all possible values of* $ac - bd$ *where a, b, c and d are digits.*

Vectorisation cont.

The brute-force solution is using explicit loops over all combinations:

```
dd.for.c <- function() {
  val <- NULL
  for (a in 0:9)
      for (b in 0:9)
          for (d in 0:9)
              for (e in 0:9)
                  val <- c(val, a*b - d*e)
  table(val)
}
```

The naive time is

```
> mean(replicate(10, system.time(dd.for.c())["elapsed"]))
```

```
[1] 0.2678
```

Vectorisation cont.

The case study discusses two important points that bear repeating:

- pre-allocating space helps with performance:
  `val <- double(10000)`
  and using `val[i <- i + 1]` as the left-hand side reduces the time to 0.1204, or less than half.
- switching to faster functions can help as well as `tabulate` outperforms `table` and reduced the time further to 0.1180.

Vectorisation cont.

However, by far the largest improvement comes from eliminating the four loops with two calls each to `outer`:

```
dd.fast.tabulate <- function() {
  val <- outer(0:9, 0:9, "*")
  val <- outer(val, val, "-")
  tabulate(val)
}
```

The time for the most efficient solution is:

```
> mean(replicate(10,
       system.time(dd.fast.tabulate())["elapsed"]))
```

```
[1] 0.0014
```

which is orders of magnitude faster than the initial naive approach.

Accelerated R with just-in-time compilation

Stephen Milborrow maintains “Ra”, a set of patches to R that allow ’just-in-time compilation’ of loops and arithmetic expressions. Together with his `jit` package on CRAN, this can be used to obtain speedups of standard R operations.

Our trivial example run in `Ra`:

```
library(jit)
sillysum <- function(N) { jit(1); s <- 0;  \
     for (i in 1:N) s <- s + i; return(s) }
```

```
 > system.time(print(sillysum(1e7)))
[1] 5e+13
   user  system elapsed
  1.548   0.028   1.577
```

which gets a speed increase of a factor of five—not bad at all.

Accelerated R with just-in-time compilation

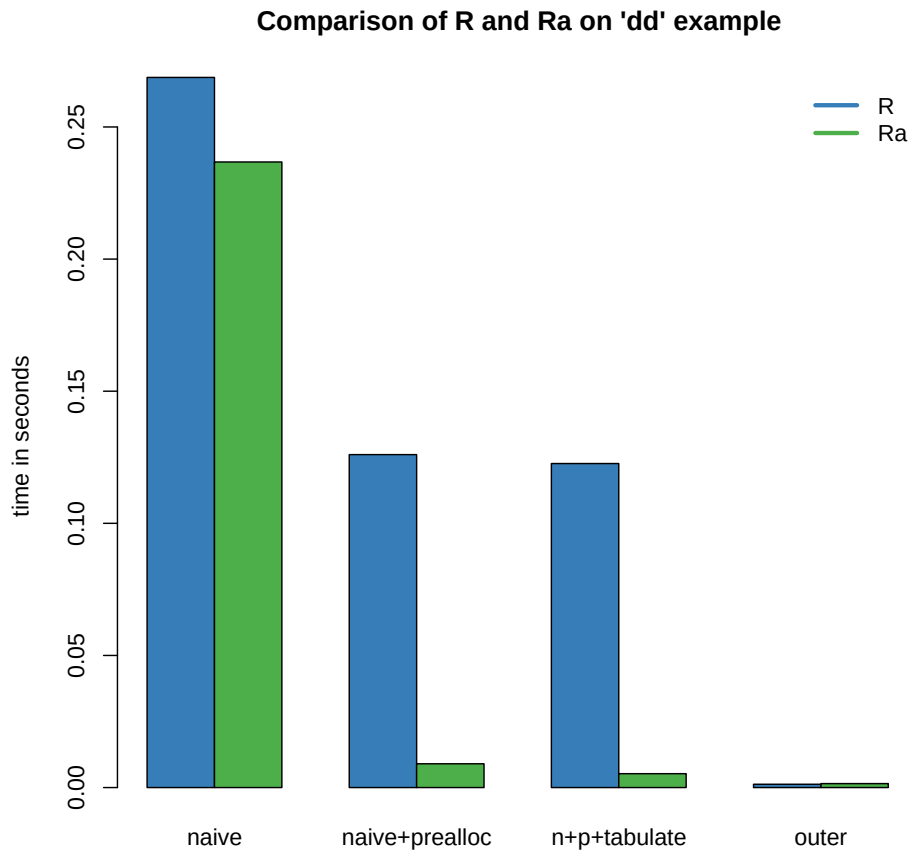
The last looping example can be improved with jit:

```
dd.for.pre.tabulate.jit <- function() {
  jit(1)
  val <- double(10000)
  i <- 0
  for (a in 0:9) for (b in 0:9)
      for (d in 0:9) for (e in 0:9) {
          val[i <- i + 1] <- a*b - d*e
  }
  tabulate(val)
}
```

```
 > mean(replicate(10, system.time(dd.for.pre.tabulate.jit())["
[1] 0.0053
```

or only about three to four times slower than the non-looped solution using 'outer'—a rather decent improvement.

Accelerated R with just-in-time compilation



Source: Our calculations

`Ra` achieves very good decreases in total computing time in these examples but cannot improve the efficient solution any further.

`Ra` and `jit` are still fairly new and not widely deployed yet, but readily available in Debian and Ubuntu.

Optimised BLAS

BLAS ('basic linear algebra subprogram') are standard building blocks for linear algebra. Highly-optimised libraries exist that can provide considerable performance gains.

R can be built using so-called optimised BLAS such as Atlas (open source), Goto (not 'free'), or the Intel MKL or AMD AMCL; see the 'R Admin' manual, section A.3 'Linear Algebra'.

The speed gains can be noticeable. For Debian/Ubuntu, one can simply install one of the `atlas-base-*` packages.

An example from the old README.Atlas, running with a R 2.8.1 on a four-core machine follow.

Optimised Blas cont.

```
# with Atlas
> mm <- matrix(rnorm(4*10^6), ncol = 2*10^3)
> mean(replicate(10,
       system.time(crossprod(mm))["elapsed"]),trim=0.1)
```

```
[1] 2.6465
```

```
# with basic. non-optmised Blas,
> mm <- matrix(rnorm(4*10^6), ncol = 2*10^3)
> mean(replicate(10,
       system.time(crossprod(mm))["elapsed"]),trim=0.1)
```

```
[1] 16.42813
```

For linear algebra problems, we may get an improvement by an integer factor that may be as large (or even larger) than the number of cores as we benefit from both better code and multithreaded execution. Even higher increases are possibly by 'tuning' the library, see the Atlas documentation.

From Blas to GPUs.

The next frontier for hardware acceleration is computing on GPUs ('graphics programming units').

GPUs are essentially hardware that is optimised for I/O and floating point operations, leading to much faster code execution than standard CPUs on floating-point operations.

The key development environments that are available are

- Nvidia CUDA (Compute Unified Device Architecture) introduced in 2007 and provides C-like programming
- OpenCL (Open Computing Language) introduced in 2009 provides a vendor-independent interface to GPU hardware.

GPU resources

These are some of the resources and libraries for GPU programming:

- Vendor-specific:
  - CUDA for NVidia hardware
  - ATI Stream SDL for AMD hardware
- Vendor-independent: OpenCL
- For CUDA / NVividia:
  - BLAS on GPUs: Magma for Multicore/GPU
  - STL-alike containers: Thrust
  - Commercial CUDA libraries: CULAtools

CUDA Example

Consider a simple vector multiplication. In C, we write

```
1  void vecMult_h(int *A, int *B, unsigned long long N) {
2      for (unsigned long long i=0;i<N;i++) {
3        B[i] = A[i]*2;
4      }
5  }
6
7  // which gets called as ...
8  a_h = (int *)malloc(sizeof(int)*n);
9  b_h = (int *)malloc(sizeof(int)*n);
10 // ... fill a_h
11 vecMult_h(a_h, b_h, n);
```

CUDA Example

With CUDA, we create so-called *kernels* which access the data in parallel using multiple threads. The equivalent function is

```
1  __global__ void vecMult_d(int *A, int *B, int N) {
2      int i = blockIdx.x * blockDim.x + threadIdx.x ;
3      if (i<N) {
4        B[i] = A[i]*2;
5      }
6  }
7
8  // which gets called as ...
9  cudaMalloc((void **)&a_d, n*sizeof(int));    // alloc. on device
10 cudaMalloc((void **)&b_d, n*sizeof(int));
11 dim3 dimBlock( blocksize );
12 dim3 dimGrid( ceil(float(n)/float(dimBlock.x)) );
13 cudaMemcpy(a_d, a_h, n*sizeof(int),cudaMemcpyHostToDevice);
14 vecMult_d<<<dimGrid,dimBlock>>>(a_d,b_d,n);
15 cudaThreadSynchronize();
16 cudaMemcpy(b_h, b_d, n*sizeof(int),cudaMemcpyDeviceToHost);
```

GPU programming for R

Currently, two packages provide GPU computing for R:

- gputools by Josh Buckner and Mark Seligman provides a number of basic routines (among them are e.g. `gpuCor`, `gpuDistClust`, `gpuFastICA`, `gpuGranger`, `gpuHclust`, `gpuLm`, `gpuMatMult`, `gpuSolve`, `gpuSvd`, `gpuSvmPredict`, `gpuSvmTrain`).
- cudaBayesreg by Adelino Ferreira da Silva reimplements Bayesian multilevel modeling for fMRI data.

Both use the CUDA toolchain for NVidia hardware.

GPU performance with R

A simple example, using a matrix of size 720 x 98 containing almost three years of daily returns data on the SP100:

```
# using R
> system.time(cor(X, method="kendall"))
# using GPU
> system.time(gpuCor(X, method="kendall"))
```

```
   user  system elapsed
  8.350   0.070   8.434
   user  system elapsed
 59.220   0.000  59.224
```

This correspond to about a *seven-fold* increase in speed.

GPU performance with R

Now let's redo the example using a matrix of size 1206 x 477 containing almost five years of daily returns data on the SP500:

```
# using R
> system.time(cor(X, method="kendall"))
# using GPU
> system.time(gpuCor(X, method="kendall"))
```

```
   user  system elapsed
148.650   0.070 148.716
    user   system  elapsed
3925.730    0.010 3925.735
```

This correspond to about a *twenty-six-fold* increase in speed!

How is GPU programming different?

As R or C/C++ programmers on modern hardware, our life is relatively easy: flat and large memory spaces, little direct consideration of hardware representation.

This makes for a nice level of abstraction.

With GPU, this abstraction goes away and we have to worry (again) about memory layout, access, ...

So while there is a clear promise of increased performance, there is clearly 'No Free Lunch'.

Outline

Compiled Code

Beyond smarter code (using *e.g.* vectorised expression and/or just-in-time compilation), hardware-driven acceleration or optimised libraries, the most direct speed gain comes from switching to compiled code.

This section covers two possible approaches:

- `inline` for automated wrapping of simple expression
- `Rcpp` for easing the interface between R and C++

A different approach is to keep the core logic 'outside' but to *embed* R into the application. There is some documentation in the 'R Extensions' manual—and the `RInside` package offers C++ classes to automate this.

This requires some familiarity with R internals though the `Rcpp` and `RInside` packages aim to hide much of this complexity.

Compiled Code: The Basics

R offers several functions to access compiled code: `.C` and `.Fortran` as well as `.Call` and `.External`. (*R Extensions*, sections 5.2 and 5.9; *Software for Data Analysis*). `.C` and `.Fortran` are older and simpler, but more restrictive in the long run.

The canonical example in the documentation is the convolution function:

```
1  void convolve(double *a, int *na, double *b,
2                int *nb, double *ab)
3  {
4    int i, j, nab = *na + *nb - 1;
5
6    for(i = 0; i < nab; i++)
7      ab[i] = 0.0;
8    for(i = 0; i < *na; i++)
9      for(j = 0; j < *nb; j++)
10       ab[i + j] += a[i] * b[j];
11 }
```

Compiled Code: The Basics cont.

The convolution function is called from R by

```
1 conv <- function(a, b)
2   .C("convolve",
3      as.double(a),
4      as.integer(length(a)),
5      as.double(b),
6      as.integer(length(b)),
7      ab = double(length(a) + length(b) - 1))$ab
```

As stated in the manual, one must take care to coerce all the arguments to the correct R storage mode before calling `.C` as mistakes in matching the types can lead to wrong results or hard-to-catch errors.

The script `convolve.C.sh` compiles and links the source code, and then calls R to run the example.

Compiled Code: The Basics cont.

Using `.Call`, the example becomes

```
1  #include <R.h>
2  #include <Rdefines.h>
3
4  SEXP convolve2(SEXP a, SEXP b)
5  {
6     int i, j, na, nb, nab;
7     double *xa, *xb, *xab;
8     SEXP ab;
9
10    PROTECT(a = AS_NUMERIC(a));
11    PROTECT(b = AS_NUMERIC(b));
12    na = LENGTH(a); nb = LENGTH(b); nab = na + nb - 1;
13    PROTECT(ab = NEW_NUMERIC(nab));
14    xa = NUMERIC_POINTER(a); xb = NUMERIC_POINTER(b);
15    xab = NUMERIC_POINTER(ab);
16    for(i = 0; i < nab; i++) xab[i] = 0.0;
17    for(i = 0; i < na; i++)
18       for(j = 0; j < nb; j++) xab[i + j] += xa[i] * xb[j];
19    UNPROTECT(3);
20    return(ab);
21 }
```

Compiled Code: The Basics cont.

Now the call becomes easier by just using the function name and the vector arguments—all other handling is done at the C/C++ level:

```
conv <- function(a, b) .Call("convolve2", a, b)
```

The script `convolve.Call.sh` compiles and links the source code, and then calls R to run the example.

In summary, we see that

- there are different entry points
- using different calling conventions
- leading to code that may need to do more work at the lower level.

Compiled Code: inline

`inline` is a package by Oleg Sklyar et al that provides the function `cfunction` that can wrap Fortran, C or C++ code.

```
## A simple Fortran example
code <- "
      integer i
      do 1 i=1, n(1)
    1 x(i) = x(i)**3
"
cubefn <- cfunction(signature(n="integer", x="numeric"),
                    code, convention=".Fortran")
x <- as.numeric(1:10)
n <- as.integer(10)
cubefn(n, x)$x
```

`cfunction` takes care of compiling, linking, loading, ... by placing the resulting dynamically-loadable object code in the per-session temporary directory used by R.

Run this via `cat inline.Fortan.R | R -no-save`.

Compiled Code: inline cont.

`inline` defaults to using the `.Call()` interface:

```
1  ## Use of .Call convention with C code
2  ## Multyplying each image in a stack with a 2D Gaussian at a given position
3  code <- "
4    SEXP res;
5    int nprotect = 0, nx, ny, nz, x, y;
6    PROTECT(res = Rf_duplicate(a)); nprotect++;
7    nx = INTEGER(GET_DIM(a))[0];
8    ny = INTEGER(GET_DIM(a))[1];
9    nz = INTEGER(GET_DIM(a))[2];
10   double sigma2 = REAL(s)[0] * REAL(s)[0], d2 ;
11   double cx = REAL(centre)[0], cy = REAL(centre)[1], *data, *rdata;
12   for (int im = 0; im < nz; im++) {
13     data = &(REAL(a)[im*nx*ny]); rdata = &(REAL(res)[im*nx*ny]);
14     for (x = 0; x < nx; x++)
15       for (y = 0; y < ny; y++) {
16         d2 = (x-cx)*(x-cx) + (y-cy)*(y-cy);
17         rdata[x + y*nx] = data[x + y*nx] * exp(-d2/sigma2);
18       }
19   }
20   UNPROTECT(nprotect);
21   return res;
22 "
23 funx <- cfunction(signature(a="array", s="numeric", centre="numeric"), code)
24
25 x <- array(runif(50*50), c(50,50,1))
26 res <- funx(a=x, s=10, centre=c(25,15))   ## actual call of compiled function
27 if (interactive()) image(res[,,1])
```

Compiled Code: inline cont.

We can revisit the earlier distribution of determinants example.

If we keep it very simple and pre-allocate the temporary vector in R , the example becomes

```
code <- "
  if (isNumeric(vec)) {
    int *pv = INTEGER(vec);
    int n = length(vec);
    if (n = 10000) {
      int i = 0;
      for (int a = 0; a < 9; a++)
        for (int b = 0; b < 9; b++)
          for (int c = 0; c < 9; c++)
            for (int d = 0; d < 9; d++)
              pv[i++] = a*b - c*d;
    }
  }
  return(vec);
"

funx <- cfunction(signature(vec="numeric"), code)
```

Compiled Code: inline cont.

We can use the inlined function in a new function to be timed:

```
dd.inline <- function() {
    x <- integer(10000)
    res <- funx(vec=x)
    tabulate(res)
}
> mean(replicate(100,system.time(dd.inline())["elapsed"]))

[1] 0.00051
```

Even though it uses the simplest algorithm, pre-allocates memory in R and analyses the result in R , it is still more than twice as fast as the previous best solution.

The script `dd.inline.r` runs this example.

Compiled Code: Rcpp

`Rcpp` makes it easier to interface C++ and R code.

Using the `.Call` interface, we can use features of the C++ language to automate the tedious bits of the macro-based C-level interface to R.

One major advantage of using `.Call` is that vectors (or matrices) can be passed directly between R and C++ without the need for explicit passing of dimension arguments. And by using the C++ class layers, we do not need to directly manipulate the SEXP objects.

So let us rewrite the 'distribution of determinant' example one more time.

Rcpp example

The simplest version can be set up as follows:

```
1  #include <Rcpp.h>
2
3  RcppExport SEXP dd_rcpp(SEXP v) {
4    SEXP  rl = R_NilValue;              // Use this when nothing is returned
5
6    RcppVector<int> vec(v);             // vec parameter viewed as vector of doubles
7    int n = vec.size(), i = 0;
8
9    for (int a = 0; a < 9; a++)
10     for (int b = 0; b < 9; b++)
11       for (int c = 0; c < 9; c++)
12         for (int d = 0; d < 9; d++)
13           vec(i++) = a*b - c*d;
14
15   RcppResultSet rs;                   // Build result set returned as list to R
16   rs.add("vec", vec);                 // vec as named element with name 'vec'
17   rl = rs.getReturnList();            // Get the list to be returned to R.
18
19   return rl;
20 }
```

but it is actually preferable to use the exception-handling feature of C++ as in the slightly longer next version.

Rcpp example cont.

```
1  #include <Rcpp.h>
2
3  RcppExport SEXP dd_rcpp(SEXP v) {
4    SEXP  rl = R_NilValue;          // Use this when there is nothing to be returned.
5    char* exceptionMesg = NULL;     // msg var in case of error
6
7    try {
8      RcppVector<int> vec(v);       // vec parameter viewed as vector of ints.
9      int n = vec.size(), i = 0;
10     if (n != 10000) throw std::length_error("Wrong vector size");
11     for (int a = 0; a < 9; a++)
12       for (int b = 0; b < 9; b++)
13         for (int c = 0; c < 9; c++)
14           for (int d = 0; d < 9; d++)
15             vec(i++) = a*b - c*d;
16
17     RcppResultSet rs;             // Build result set to be returned as a list to R.
18     rs.add("vec", vec);           // vec as named element with name 'vec'
19     rl = rs.getReturnList();      // Get the list to be returned to R.
20   } catch(std::exception& ex) {
21     exceptionMesg = copyMessageToR(ex.what());
22   } catch(...) {
23     exceptionMesg = copyMessageToR("unknown reason");
24   }
25
26   if (exceptionMesg != NULL) Rf_error(exceptionMesg);
27
28   return rl;
29 }
```

Rcpp example cont.

We can create a shared library from the source file as follows:

```
PKG_CPPFLAGS=`r -e'Rcpp:::CxxFlags()'` \
     PKG_LIBS=`r -e'Rcpp:::LdFlags()'` \
     R CMD SHLIB dd.rcpp.cpp
```

```
g++ -I/usr/share/R/include \
     -I/usr/lib/R/site-library/Rcpp/lib \
     -fpic -g -O2 \
     -c dd.rcpp.cpp -o dd.rcpp.o
g++ -shared -o dd.rcpp.so dd.rcpp.o \
     -L/usr/lib/R/site-library/Rcpp/lib \
     -lRcpp -Wl,-rpath,/usr/lib/R/site-library/Rcpp/lib \
     -L/usr/lib/R/lib -lR
```

Note how we let the `Rcpp` package tell us where header and library files are stored.

Rcpp example cont.

We can then load the file using `dyn.load` and proceed as in the `inline` example.

```
dyn.load("dd.rcpp.so")

dd.rcpp <- function() {
    x <- integer(10000)
    res <- .Call("dd_rcpp", x)
    tabulate(res$vec)
}

mean(replicate(100,system.time(dd.rcpp())["elapsed"]))
```

```
[1] 0.00047
```

This beats the `inline` example by a neglible amount which is probably due to some overhead in the easy-to-use inlining.

The file `dd.rcpp.sh` runs the full Rcpp example.

Basic Rcpp usage

`Rcpp` eases data transfer from R to C++, and back. We always convert to and from `SEXP`, and return a `SEXP` to R.

The key is that we can consider this to be a 'variant' type permitting us to extract using appropriate C++ classes. We pass data from R via named lists that may contain different types:

```
list(intnb=42, fltnb=6.78, date=Sys.Date(),
     txt="some thing", bool=FALSE)
```

by initialising a `RcppParams` object and extracting as in

```
RcppParams param(inputsexp);
int      nmb = param.getIntValue("intnb");
double   dbl = param.getDoubleValue("fltnb");
string   txt = param.getStringValue("txt");
bool     flg = param.getBoolValue("bool";
RcppDate dt  = param.getDateValue("date");
```

Basic Rcpp usage (cont.)

Similarly, we can constructs vectors and matrics of `double`, `int`, as well as vectors of types `string` and date and datetime. The key is that we *never* have to deal with dimensions and / or memory allocations — all this is shielded by C++ classes.

Similarly, for the return, we declare an object of type `RcppResultSet` and use the `add` methods to insert named elements before coverting this into a list that is assigned to the returned `SEXP`.

Back in R, we access them as elements of a standard R list by position or name.

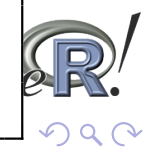
Another Rcpp example

Let us revisit the `lm()` versus `lm.fit()` example. How fast could compiled code be? Let's wrap a GNU GSL function.

```
1  #include <cstdio>
2  extern "C" {
3  #include <gsl/gsl_multifit.h>
4  }
5  #include <Rcpp.h>
6
7  RcppExport SEXP gsl_multifit(SEXP Xsexp, SEXP Ysexp) {
8      SEXP rl=R_NilValue;
9      char *exceptionMesg=NULL;
10
11     try {
12         RcppMatrixView<double> Xr(Xsexp);
13         RcppVectorView<double> Yr(Ysexp);
14
15         int i,j,n = Xr.dim1(), k = Xr.dim2();
16         double chisq;
17
18         gsl_matrix *X = gsl_matrix_alloc (n, k);
19         gsl_vector *y = gsl_vector_alloc (n);
20         gsl_vector *c = gsl_vector_alloc (k);
21         gsl_matrix *cov = gsl_matrix_alloc (k, k);
22         for (i = 0; i < n; i++) {
23             for (j = 0; j < k; j++)
24                 gsl_matrix_set (X, i, j, Xr(i,j));
25             gsl_vector_set (y, i, Yr(i));
26         }
```

Another Rcpp example (cont.)

```
27          gsl_multifit_linear_workspace *work = gsl_multifit_linear_alloc (n, k);
28          gsl_multifit_linear (X, y, c, cov, &chisq, work);
29          gsl_multifit_linear_free (work);
30
31          RcppMatrix<double> CovMat(k, k);
32          RcppVector<double> Coef(k);
33          for (i = 0; i < k; i++) {
34              for (j = 0; j < k; j++)
35                  CovMat(i,j) = gsl_matrix_get(cov,i,j);
36              Coef(i) = gsl_vector_get(c,i);
37          }
38          gsl_matrix_free (X);
39          gsl_vector_free (y);
40          gsl_vector_free (c);
41          gsl_matrix_free (cov);
42
43          RcppResultSet rs;
44          rs.add("coef", Coef);
45          rs.add("covmat", CovMat);
46
47          rl = rs.getReturnList();
48
49      } catch(std::exception& ex) {
50          exceptionMesg = copyMessageToR(ex.what());
51      } catch(...) {
52          exceptionMesg = copyMessageToR("unknown reason");
53      }
54      if(exceptionMesg != NULL) Rf_error(exceptionMesg);
55      return rl;
56  }
```



Another Rcpp example (cont.)

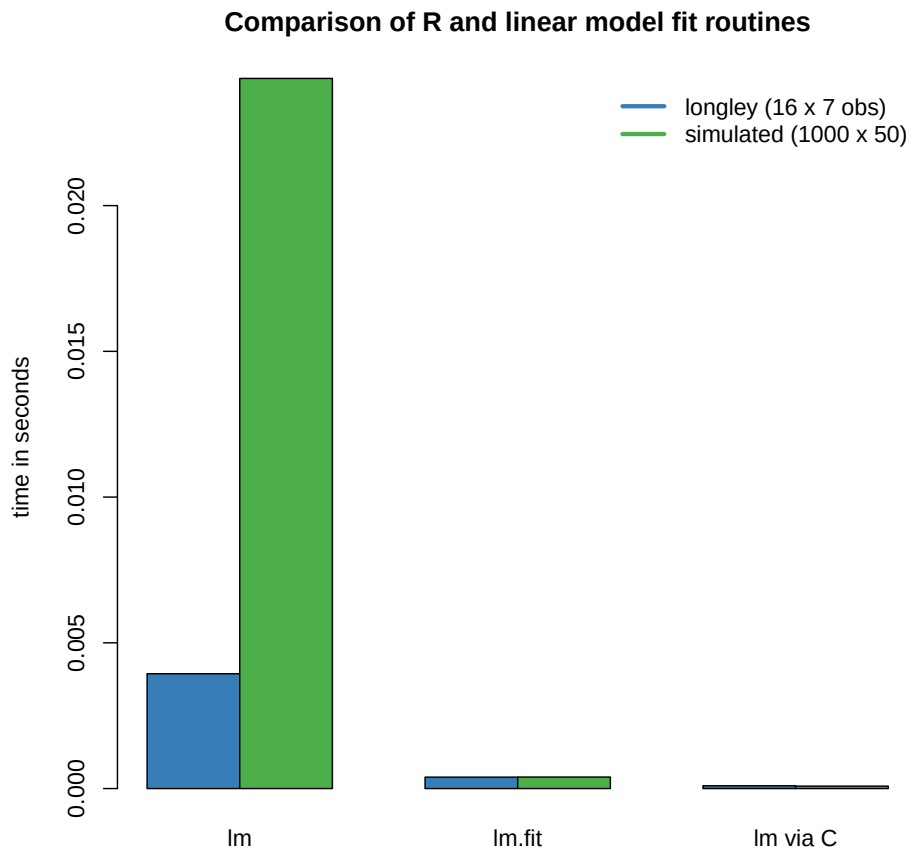
We can build a shared library for R via

```
RCPP_CXXFLAGS=`Rscript -e 'Rcpp:::CxxFlags()'`
RCPP_LIBS=`Rscript -e 'Rcpp:::LdFlags()'`

PKG_CPPFLAGS="-W ${RCPP_CXXFLAGS}" \
    PKG_LIBS="-lgsl -lblas ${RCPP_LIBS}" \
    R CMD SHLIB gsl_multifit_in_R.cpp
```

and run the example code via

```
dyn.load("gsl_multifit_in_R.so")
## generate X and y
N <- 100
mean(replicate(N, system.time(val <-
    .Call("gsl_multifit", X, y))["elapsed"]),trim=0.05)
```

Another Rcpp example (cont.)

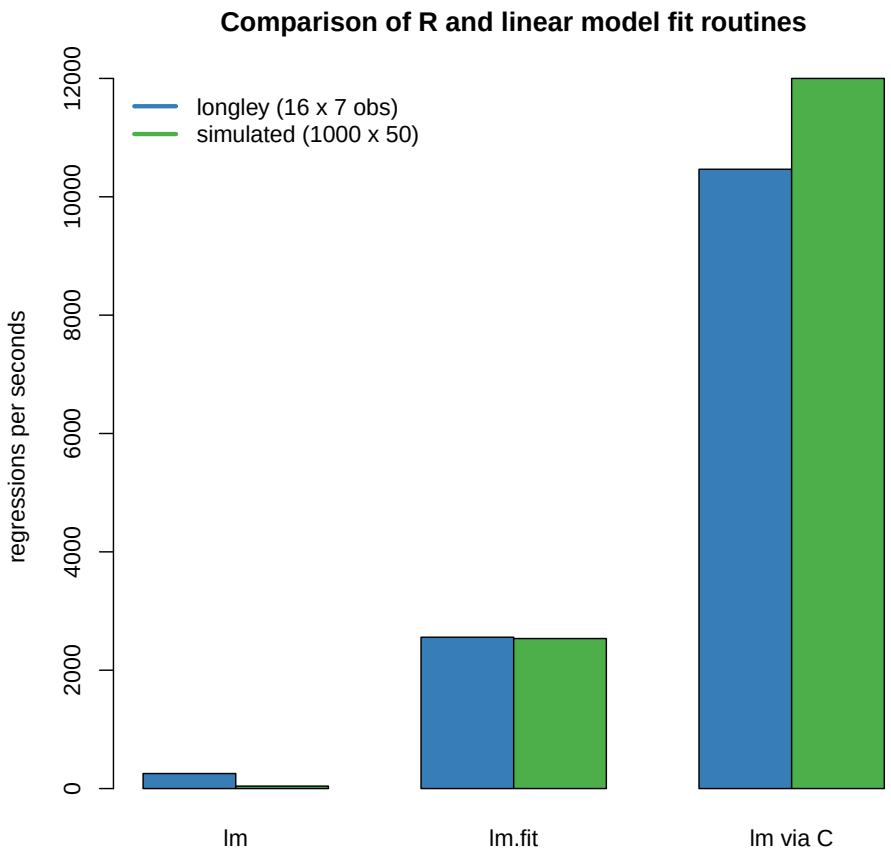


Source: Our calculations

The small `longley` example exhibits less variability between methods, but the larger data set shows the gains more clearly.

The `lm.fit()` approach appears unchanged between `longley` and the larger simulated data set.

Another Rcpp example (cont.)



Source: Our calculations

By inverting the times to see how many 'regressions per second' we can fit, the merits of the compiled code become clearer.

One caveat, measurements depends critically on the size of the data as well as the cpu and libraries that are used.

Revisiting profiling

We can also use the preceding example to illustrate how to profile subroutines.

We can add the following to the top of the function:

```
ProfilerStart("/tmp/ols.profile");
for (unsigned int i=1; i<10000; i++) {
```

and similarly

```
}
ProfilerStop();
```

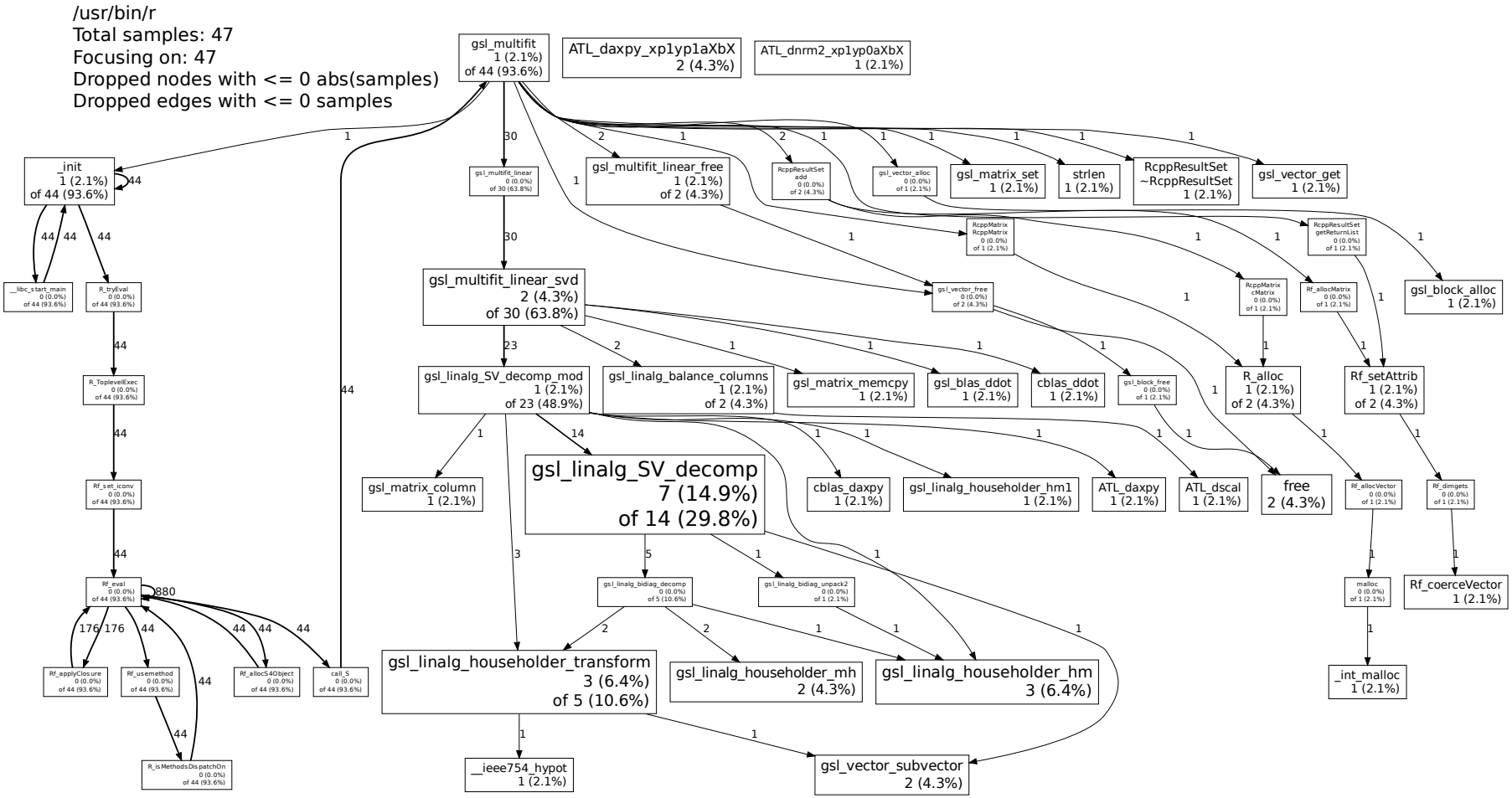
at end before returning. If we then call this function just once from R as in

```
print(system.time(invisible(val <-
      .Call("gsl_multifit", X, y))))
```

we can then call the profiling tools on the output:

```
google-pprof --gv /usr/bin/r /tmp/ols.profile
```

Revisiting profiling



Rcpp and package building

Two tips for easing builds with `Rcpp`:

For command-line use, a shortcut is to copy `Rcpp.h` to `/usr/local/include`, and `libRcpp.so` to `/usr/local/lib`. The earlier example reduces to

```
R CMD SHLIB dd.rcpp.cpp
```

as header and library will be found in the default locations.

For package building, we can have a file `src/Makevars` with

```
# compile flag providing header directory
PKG_CXXFLAGS=`Rscript -e 'Rcpp:::CxxFlags()'`
# link flag providing libary and path
PKG_LIBS=`Rscript -e 'Rcpp:::LdFlags()'`
```

See `help(Rcpp-package)` for more details.

RInside and bringing R to C++

Sometimes we may want to go the other way and add R to and existing C++ project.

This can be simplified using `RInside`:

```
1  #include "RInside.h"                    // for the embedded R via RInside
2  #include "Rcpp.h"                       // for the R / Cpp interface
3
4  int main(int argc, char *argv[]) {
5
6      RInside R(argc, argv);              // create an embedded R instance
7
8      std::string txt = "Hello, world!\n";// assign a standard C++ string to 'txt'
9      R.assign( txt, "txt");              // assign string var to R variable 'txt'
10
11     std::string evalstr = "cat(txt)";
12     R.parseEvalQ(evalstr);              // eval the init string, ignoring any returns
13
14     exit(0);
15 }
```

RInside and bringing R to C++ (cont)

```
1  #include "RInside.h"                    // for the embedded R via RInside
2  #include "Rcpp.h"                       // for the R / Cpp interface used for transfer
3
4  std::vector< std::vector< double > > createMatrix(const int n) {
5      std::vector< std::vector< double > > mat;
6      for (int i=0; i<n; i++) {
7          std::vector<double> row;
8          for (int j=0; j<n; j++) row.push_back((i*10+j));
9          mat.push_back(row);
10     }
11     return(mat);
12 }
13
14 int main(int argc, char *argv[]) {
15     const int mdim = 4;
16     std::string evalstr = "cat('Running ls()\n'); print(ls()); \
17         cat('Showing M\n'); print(M); cat('Showing colSums()\n'); \
18         Z <- colSums(M); print(Z); Z";  ## returns Z
19     RInside R(argc, argv);
20     SEXP ans;
21     std::vector< std::vector< double > > myMatrix = createMatrix(mdim);
22     R.assign( myMatrix, "M");              // assign STL matrix to R's 'M' var
23     R.parseEval(evalstr, ans);             // eval the init string -- Z is now in ans
24     RcppVector<double> vec(ans);           // now vec contains Z via ans
25     vector<double> v = vec.stlVector();    // convert RcppVector to STL vector
26     for (unsigned int i=0; i< v.size(); i++)
27         std::cout << "In C++ element " << i << " is " << v[i] << std::endl;
28     exit(0);
29 }
```

Debugging example: valgrind

Analysis of compiled code is mainly undertaken with a debugger like `gdb`, or a graphical frontend like `ddd`.

Another useful tool is `valgrind` which can find memory leaks. We can illustrate its use with a recent real-life example.

`RMySQL` had recently been found to be leaking memory when database connections are being established and closed. Given how `RPostgreSQL` shares a common heritage, it seemed like a good idea to check.

Debugging example: valgrind

We create a small test script which opens and closes a connection to the database in a loop and sends a small 'select' query. We can run this in a way that is close to the suggested use from the 'R Extensions' manual:

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

which creates copious output, including what is on the next slide.

Given the source file and line number, it is fairly straightforward to locate the source of error: a vector of pointers was freed without freeing the individual entries first.

Debugging example: valgrind

The state before the fix:

```
[...]
#==21642== 2,991 bytes in 299 blocks are definitely lost in loss record 34 of 47
#==21642==    at 0x4023D6E: malloc (vg_replace_malloc.c:207)
#==21642==    by 0x6781CAF: RS_DBI_copyString (RS-DBI.c:592)
#==21642==    by 0x6784B91: RS_PostgreSQL_createDataMappings (RS-PostgreSQL.c:400)
#==21642==    by 0x6785191: RS_PostgreSQL_exec (RS-PostgreSQL.c:366)
#==21642==    by 0x40C50BB: (within /usr/lib/R/lib/libR.so)
#==21642==    by 0x40EDD49: Rf_eval (in /usr/lib/R/lib/libR.so)
#==21642==    by 0x40F00DC: (within /usr/lib/R/lib/libR.so)
#==21642==    by 0x40EDA74: Rf_eval (in /usr/lib/R/lib/libR.so)
#==21642==    by 0x40F0186: (within /usr/lib/R/lib/libR.so)
#==21642==    by 0x40EDA74: Rf_eval (in /usr/lib/R/lib/libR.so)
#==21642==    by 0x40F16E6: Rf_applyClosure (in /usr/lib/R/lib/libR.so)
#==21642==    by 0x40ED99A: Rf_eval (in /usr/lib/R/lib/libR.so)
#==21642==
#==21642== LEAK SUMMARY:
#==21642==    definitely lost: 3,063 bytes in 301 blocks.
#==21642==    indirectly lost: 240 bytes in 20 blocks.
#==21642==      possibly lost: 9 bytes in 1 blocks.
#==21642==    still reachable: 13,800,378 bytes in 8,420 blocks.
#==21642==         suppressed: 0 bytes in 0 blocks.
#==21642== Reachable blocks (those to which a pointer was found) are not shown.
#==21642== To see them, rerun with: --leak-check=full --show-reachable=yes
```

Debugging example: valgrind

The state after the fix:

```
[...]
#==3820==
#==3820== 312 (72 direct, 240 indirect) bytes in 2 blocks are definitely lost in loss record
#==3820==    at 0x4023D6E: malloc (vg_replace_malloc.c:207)
#==3820==    by 0x43F1563: nss_parse_service_list (nsswitch.c:530)
#==3820==    by 0x43F1CC3: __nss_database_lookup (nsswitch.c:134)
#==3820==    by 0x445EF4B: ???
#==3820==    by 0x445FCEC: ???
#==3820==    by 0x43AB0F1: getpwuid_r@@GLIBC_2.1.2 (getXXbyYY_r.c:226)
#==3820==    by 0x43AAA76: getpwuid (getXXbyYY.c:116)
#==3820==    by 0x4149412: (within /usr/lib/R/lib/libR.so)
#==3820==    by 0x412779D: (within /usr/lib/R/lib/libR.so)
#==3820==    by 0x40EDA74: Rf_eval (in /usr/lib/R/lib/libR.so)
#==3820==    by 0x40F00DC: (within /usr/lib/R/lib/libR.so)
#==3820==    by 0x40EDA74: Rf_eval (in /usr/lib/R/lib/libR.so)
#==3820==
#==3820== LEAK SUMMARY:
#==3820==    definitely lost: 72 bytes in 2 blocks.
#==3820==    indirectly lost: 240 bytes in 20 blocks.
#==3820==      possibly lost: 0 bytes in 0 blocks.
#==3820==    still reachable: 13,800,378 bytes in 8,420 blocks.
#==3820==         suppressed: 0 bytes in 0 blocks.
#==3820== Reachable blocks (those to which a pointer was found) are not shown.
#==3820== To see them, rerun with: --leak-check=full --show-reachable=yes
```

showing that we recovered 3000 bytes.

Outline

Embarassingly parallel

Several CRAN (or R-Forge) packages provide the ability to execute R code in parallel:

- `NWS`
- `Rmpi`
- `snow` (using MPI, PVM, NWS or sockets)
- `multicore`
- `foreach` with `doMC`, `doSNOW`, `doMPI`
- plus several others (`rpvm`, `papply`, `taskPR` ...)

The paper by Schmidberger, Morgan, Eddelbuettel, Yu, Tierney and Mansmann (JSS, 2009) provides a survey.

NWS Intro

NWS ("NetWorkSpaces") is an alternative to MPI (see below). It is based on Python and cross-platform. NWS is accessible from R, Python, Matlab, Ruby, and other languages.

NWS is available via Sourceforge and CRAN. An introductory article appeared in Dr. Dobb's.

On Debian and Ubuntu, installing the `python-nwsserver` package on at least the server node, and installing `r-cran-nws` on each client is all that is needed. Other systems may need to install the `twisted` framework for `Python` first.

NWS data store example

A simple example, adapted from `demo(nwsExample)`

```
ws <- netWorkSpace('r place') # create a 'value store'
nwsStore(ws, 'x', 1)          # place a value (as fifo)

cat(nwsListVars(ws), "\n")    # we can list
nwsFind(ws, 'x')              # and lookup
nwsStore(ws, 'x', 2)          # and overwrite
cat(nwsListVars(ws), "\n")    # now see two entries

cat(nwsFetch(ws, 'x'), '\n')  # we can fetch
cat(nwsFetch(ws, 'x'), '\n')  # we can fetch
cat(nwsListVars(ws), '\n')    # and none left

cat(nwsFetchTry(ws,'x','no go'),'\n') # can't fetch
```

NWS sleigh example

The NWS component sleigh is an R class that makes it easy to write simple parallel programs. Sleigh uses the master / worker paradigm: The master submits tasks to the workers, who may or may not be on the same machine as the master.

```
# create a sleigh object on two nodes using ssh
s <- sleigh(nodeList=c("joe", "ron"), launch=sshcmd)

# execute a statement on each worker node
eachWorker(s, function() x <<- 1)

# get system info from each worker
eachWorker(s, Sys.info)

# run a lapply-style funct. over each list elem.
eachElem(s, function(x) {x+1}, list(1:10))

stopSleigh(s)
```

NWS sleigh cont.

Also of note is the extended `caretNWS` version of `caret` by Max Kuhn, and described in a recent JSS article.

`caret` (short for 'Classification and Regression Training') provides a consistent interface for dozens of modern regression and classification techniques.

`caretNWS` uses `nws` and `sleigh` to exeeute embarassingly parallel task: bagging, boosting, cross-validation, bootstrapping, ... This is all done 'behind the scenes' and thus easy to deploy.

Schmidberger et al find NWS to be competitive with the other parallel methods for non-degenerate cases where the ratio between communication and computation is balanced.

Rmpi

`Rmpi` is a CRAN package that provides an interface between R and the Message Passing Interface (MPI), a standard for parallel computing. (c.f. Wikipedia for more and links to the Open MPI and MPICH2 projects for implementations).

The preferred implementation for MPI is now Open MPI. However, the older LAM implementation can be used on those platforms where Open MPI is unavailable. There is also an alternate implementation called MPICH2. Lastly, we should also mention the similar Parallel Virtual Machine (PVM) tool; see its Wikipedia page for more.

`Rmpi` allows us to use MPI directly from R and comes with several examples. However, we will focus on the higher-level usage via `snow`.

MPI Example

Let us look at the MPI variant of the 'Hello, World!' program:

```
1  #include <stdio.h>
2  #include "mpi.h"
3
4  int main(int argc, char** argv)
5  {
6      int rank, size, nameLen;
7      char processorName[MPI_MAX_PROCESSOR_NAME];
8
9      MPI_Init(&argc, &argv);
10     MPI_Comm_rank(MPI_COMM_WORLD, &rank);
11     MPI_Comm_size(MPI_COMM_WORLD, &size);
12
13     MPI_Get_processor_name(processorName, &nameLen);
14
15     printf("Hello, rank %d, size %d on processor %s\n",
16            rank, size, processorName);
17
18     MPI_Finalize();
19     return 0;
20 }
```

MPI Example: cont.

We can compile the previous example via

```
$ mpicc -o mpiHelloWorld mpiHelloWorld.c
```

If it it has been copied across several Open MPI-equipped hosts, we can execute it *N* times on the *M* listed hosts via:

```
$ orterun -H ron,joe,tony,mccoy -n 8 /tmp/mpiHelloWorld

Hello, rank 0, size 8 on processor ron
Hello, rank 4, size 8 on processor ron
Hello, rank 7, size 8 on processor mccoy
Hello, rank 3, size 8 on processor mccoy
Hello, rank 2, size 8 on processor tony
Hello, rank 5, size 8 on processor joe
Hello, rank 6, size 8 on processor tony
Hello, rank 1, size 8 on processor joe
```

Notice how the order of execution is indeterminate.

MPI Example: cont.

Besides `orterun` (which replaces the `mpirun` command used by other MPI implementations), Open MPI also supplies `ompi_info` to query parameter settings.

Open MPi has very fine-grained configuration options that permit e.g. attaching particular jobs to particular cpus or cores.

Detailed documentation is provided at the web site `http://www.openmpi.org`.

We will concentrate on using MPI via the `Rmpi` package.

Rmpi

`Rmpi`, a CRAN package by Hao Yu, wraps many of the MPI API calls for use by R.

The preceding example can be rewritten in R as

```
1 #!/usr/bin/env r
2
3 library(Rmpi) # calls MPI_Init
4
5 rk <- mpi.comm.rank(0)
6 sz <- mpi.comm.size(0)
7 name <- mpi.get.processor.name()
8 cat("Hello, rank", rk, "size", sz, "on", name, "\n")
```

Rmpi: cont.

```
$ orterun -H ron,joe,tony,mccoy -n 8 \
/tmp/mpiHelloWorld.r
```

```
Hello, rank 4 size 8 on ron
Hello, rank 0 size 8 on ron
Hello, rank 3 size 8 on mccoy
Hello, rank 7 size 8 on mccoy
Hello, rank Hello, rank 21 size 8  on joe
size 8 on tony
Hello, rank 6 size 8 on tony
Hello, rank 5 size 8 on joe
```

Rmpi: cont.

We can also exectute this as a one-liner using `r` (which we discuss later):

```
$ orterun -n 8 -H ron,joe,tony,mccoy \
      r -lRmpi -e'cat("Hello", \
      mpi.comm.rank(0), "of", \
      mpi.comm.size(0), "on", \
      mpi.get.processor.name(), "\n");
      mpi.quit()'
```

```
Hello 4 of 8 on ron
Hello 3 of 8 on mccoy
Hello 7 of 8 on mccoy
Hello 0 of 8 on ron
HelloHello 2 of 8 on tony
 Hello 1 of 8 on joe
Hello 5 of 8 on joe
6 of 8 on tony
```

Rmpi: cont.

`Rmpi` offers a large number functions, mirroring the rich API provided by MPI.

`Rmpi` also offers extensions specific to working with R and its objects, including a set of `apply`-style functions to spread load across the worker nodes.

However, we will use `Rmpi` mostly indirectly via `snow`, or via the new `doMPI` package.

snow

The `snow` package by Tierney et al provides a convenient abstraction directly from R.

It can be used to initialize and use a compute cluster using one of the available methods direct socket connections, MPI, PVM, or (since the most recent release), NWS. We will focus on MPI.

A simple example:

```
cl <- makeCluster(4, "MPI")
print(clusterCall(cl, function() \
          Sys.info()[c("nodename","machine")]))
stopCluster(cl)
```

which we can as a one-liner as shown on the next slide.

snow: Example

```
$ orterun -n 1 -H ron,joe,tony,mccoy r -lsnow,Rmpi \
    -e'cl <- makeCluster(4, "MPI"); \
       res <- clusterCall(cl, \
         function() Sys.info()["nodename"]); \
       print(do.call(rbind,res)); \
       stopCluster(cl); mpi.quit()'

       4 slaves are spawned successfully. 0 failed.
     nodename
[1,] "joe"
[2,] "tony"
[3,] "mccoy"
[4,] "ron"
```

Note that we told `orterun` to start on only one node – as `snow` then starts four instances (which are split evenly over the four given hosts).

snow: Example cont.

The power of `snow` lies in the ability to use the `apply`-style paradigm over a cluster of machines:

```
params <- c("A", "B", "C", "D", "E", "F", "G", "H")
cl <- makeCluster(4, "MPI")
res <- parSapply(cl, params, \
                 FUN=function(x) myBigFunction(x))
```

will 'unroll' the parameters `params` one-each over the function argument given, utilising the cluster `cl`. In other words, we will be running four copies of `myBigFunction()` at once.

So the `snow` package provides a unifying framework for parallelly executed `apply` functions.

We will come back to more examples with `snow` below.

papply, biopara and taskPR

We saw that `Rmpi` and `NWS` have `apply`-style functions, and that `snow` provides a unified layer. `papply` is another CRAN package that wraps around `Rmpi` to distribute processing of apply-style functions across a cluster.

However, using the Open MPI-based `Rmpi` package, I was not able to get `papply` to actually successfully distribute – and retrieve – results across a cluster. So `snow` remains the preferred wrapper.

`biopara` is another package to distribute load across a cluster using direct socket-based communication. We consider `snow` to be a more general-purpose package for the same task.

`taskPR` uses the `MPI` protocol directly rather than via `Rmpi`. It is however hard-wired to use LAM and failed to launch under the Open MPI-implementation.

multicore

The `multicore` package by Simon Urbanek is a fairly recent addition to CRAN.

It provides a convenient interface to *locally* running parallel computations in R on machines with multiple cores or CPUs. Jobs can share the entire initial workspace. This is implemented using the `fork` system call available for POSIX-compliant system (*i.e.* Linux and OS X but not Windows).

All jobs launched by `multicore` share the full state of R when spawned, no data or code needs to be initialized. This make the actual spawning very fast since no new R instance needs to be started.

multicore

The `multicore` package provides two main interfaces:

- `mclapply`, a parallel / multicore version of `lapply`
- the functions `parallel` and `collect` to launch parallel execution and gather results at end

For setups in which a sufficient number of cores is available without requiring network traffic, `multicore` is likely to be a very compelling package.

Given that future cpu generation will offer 16, 32 or more cores, this package may become increasingly popular.

One thing to note is that 'anything but Windows' is required to take advantage of `multicore`.

multicore cont.

We can illustrate the `mclapply` function with a simple example:

```
R> system("pgrep R")

28352

R> mclapply(1:2,
+> FUN=function(x) system("pgrep R", intern=TRUE))

[[1]]
[1] "28352" "31512" "31513"

[[2]]
[1] "28352" "31512" "31513"
```

So two new R processes were started by `multicore`.

Iterators, foreach and dopar

REvolution Computing released several packages to CRAN to elegantly work with serial or parallel loops:

- `iterators`
- `foreach`
- backends for `%dopar%` `doMC` (for multicore) and `doSNOW` (for `snow`)

Another backend package, `doMPI` for `Rmpi`, is currently under active development and should be on CRAN in due course.

iterators

`iterators` provides an object that offers one data element at a time by calling a method `nextElem`

`iterators` can be created using the `iter` method on `list`, `vector`, `matrix`, or `data.frame` objects

`iterators` resemble the Java and Python constructs of the same name.

`iterators` are memory-friendly: one element at a time whereas sequences gets enumerated fully.

foreach

The `foreach` package provides a new looping construct which scan switch transparently between serial and parallel modes.

It can be seen a mix of `for` loops and `lapply`-style functional operation, and similar to `foreach` operators in other programming languages.

We can switch `foreach` to execute in parallel leaning on the existing `snow` or `multicore` (and soon `Rmpi`) backends

It works like `lapply`, but without the need for a function:

```
x <- foreach(i=1:10) %do% {
    sqrt(i)
}
```

and we can switch to `%dopar%` for parallel execution.

Why is this interesting?

Objects used in the body of `foreach` are automatically exported to remote nodes easing parallel programming:

```
m <- matrix(rnorm(16), 4, 4)
foreach(i=1:ncol(m)) %dopar% {
    mean(m[,i])    # makes m available on nodes
}
```

We can nest this using the `:` operator:

```
foreach (i=1:3, .combine=cbind) %:%
    foreach (j=1:3, .combine=c) %dopar%
        (i+j)
```

foreach example: demo(sincSEQ)

```
1  library(foreach)
2  # function that creates an iterator that returns subvectors
3  ivector <- function(x, chunks) {
4    n <- length(x); i <- 1
5    nextEl <- function() {
6      if (chunks <= 0 || n <= 0) stop('StopIteration')
7      m <- ceiling(n / chunks); r <- seq(i, length=m)
8      i <<- i + m; n <<- n - m; chunks <<- chunks - 1; x[r]
9    }
10   obj <- list(nextElem=nextEl)
11   class(obj) <- c('abstractiter', 'iter');   obj
12 }
13 x <- seq(-10, 10, by=0.1) # Define coordinate grid
14 cat('Running sequentially\n'); ntasks <- 4
15 # Compute the value of the sinc function at each grid point
16 z <- foreach(y=ivector(x, ntasks), .combine=cbind) %do% {
17   y <- rep(y, each=length(x));  r <- sqrt(x ^ 2 + y ^ 2)
18   matrix(10 * sin(r) / r, length(x))
19 }
20 # Plot the results as a perspective plot
21 persp(x,x,z,ylab='y',theta=30,phi=30,expand=0.5,col="lightblue")
```

foreach example: demo(sincSEQ) cont.

The key in the `foreach` demo was the line

```
z <- foreach(y=ivector(x,ntasks),.combine=cbind) %do% {
    y <- rep(y, each=length(x))
    r <- sqrt(x ^ 2 + y ^ 2)
    matrix(10 * sin(r) / r, length(x))
}
```

where *z* is computed in a `foreach` loop using a custom `ivector` iterator over the grid *x* with a given number of task; results are recombined using `cbind`.

The actual work is being done in the code block following `%do%`.

foreach example: demo(sincMC)

In order to run this code in parallel using `multicore`, we simply use

```
library(doMC)
registerDoMC()
[...]
nw <- getDoParWorkers()
cat(sprintf('Running with %d worker(s)\n', nw))
[...]
z <- foreach(y=ivector(x, nw), \
             .combine=cbind) %dopar% {
[...]
```

as can be seen via `demo(sincMC)`.

foreach example: demo(sincMPI)

Similarly, in order to run this code in parallel using `Rmpi`, we simply use the `doMPI` package (on R-Forge, soon on CRAN):

```
library(doMPI)

# create and register a doMPI cluster
cl <- startMPIcluster(count=2)
registerDoMPI(cl)
[...]
# compute the sinc function in parallel
v <- foreach(y=x, .combine="cbind") %dopar% {
  r <- sqrt(x^2 + y^2) + .Machine$double.eps
  sin(r) / r
}
[...]
closeCluster(cl)
```

as can be seen via `demo(sincMPI)`.

Using all those cores

Multi-core hardware is now a default, and the number of cores per cpus is expected to increase dramaticlly over the next few years. It is therefore becoming more important for software to take advantage of these features.

Two recent (and still 'experimental') packages by Luke Tierney are addressing this question:

- `pnmath` uses OpenMP compiler directives for parallel code;
- `pnmath0` uses pthreads and implements the same interface.

They can be found at `http://www.stat.uiowa.edu/~luke/R/experimental/`

Other (related) approaches are of course `multicore` discussed above as well as GPU computing.

pnmath and pnmath0

Both `pnmath` and `pnmath0` provide parallelized vector math functions and support routines.

Upon loading either package, a number of vector math functions are replaced with versions that are parallelized. The functions will be run using multiple threads if their results will be long enough for the parallel overhead to be outweighed by the parallel gains. On load a calibration calculation is carried out to asses the parallel overhead and adjust these thresholds.

Profiling is probably the best way to assess the possible usefulness. As a quick illustration, we compute the `qtukey` function on a eight-core machine:

pnmath and pnmath0 illustration

```
$ r -e'N=1e3;print(system.time(qtukey(seq(1,N)/N,2,2)))'

   user  system elapsed
 66.590   0.000  66.649

$ r -lpnmath -e'N=1e3; \
print(system.time(qtukey(seq(1,N)/N,2,2)))'

   user  system elapsed
 67.580   0.080   9.938

$ r -lpnmath0 -e'N=1e3; \
print(system.time(qtukey(seq(1,N)/N,2,2)))'

   user  system elapsed
 68.230   0.010   9.983
```

The 6.7-fold reduction in 'elapsed' time shows that the multithreaded version takes advantage of the 8 available cores at a sub-linear fashion as some communications overhead is involved.

These improvements will likely be folded into future R versions.

slurm resource management and queue system

Once the number of compute nodes increases, it becomes important to be able to allocate and manage resources, and to queue and batch jobs. A suitable tool is `slurm`, an open-source resource manager for Linux clusters.

Paraphrasing from the slurm website:

- it allocates exclusive and/or non-exclusive access to resources (computer nodes) to users;
- it provides a framework for starting, executing, and monitoring (typically parallel) work on a set of allocated nodes.
- it arbitrates contention for resources by managing a queue of pending work.

Slurm is being developed by a consortium including LLNL, HP, Bull, and Linux Networks.

slurm example

Slurm is rather rich in features; we will only scratch the surface here.

Slurm can use many underlying message passing / communications protocols, and MPI is well supported.

In particular, Open MPI works well with slurm. That is an advantage inasmuch as it permits use of `Rmpi`.

slurm example

A simple example:

```
$ srun -N 2 r -lRmpi -e'cat("Hello", \
      mpi.comm.rank(0), "of", \
      mpi.comm.size(0), "on", \
      mpi.get.processor.name(), "\n")'

Hello 0 of 1 on ron
Hello 0 of 1 on joe
$ srun -n 4 -N 2 -O r -lRmpi -e'cat("Hello", \
mpi.comm.rank(0), "of", \
        mpi.comm.size(0), "on", \
        mpi.get.processor.name(), "\n")'

Hello 0 of 1 on ron
Hello 0 of 1 on ron
Hello 0 of 1 on joe
Hello 0 of 1 on joe
```

This shows how to *overcommit* jobs per node, and provides an example where we set the number of worker instances on the command-line.

slurm example

Additional coomand-line tools of interest are `salloc`, `sbatch`, `scontrol`, `squeue`, `scancel` and `sinfo`. For example, to see the status of a compute cluster:

```
$ sinfo
```

```
PARTITION AVAIL  TIMELIMIT NODES  STATE NODELIST
debug*       up   infinite     2   idle mccoy,ron
```

This shows two idle nodes in a partition with the default name 'debug'.

The `sview` graphical user interface combines the functionality of a few of the command-line tools.

A more complete example will be provided below.

Use scripting with r and slurm

As discussed at the beginning, the `r` command of the `littler` package (as well as R's `Rscript`) provide more robust alternatives to 'batch' of R.

We saw that `r` can also be used four different ways:

- `r file.R`
- `echo "commands" | r`
- `r -lRmpi -e 'cat("Hello", mpi.get.processor.name())'`
- and *shebang*-style in script files: `#!/usr/bin/r`

It is the last point that is of particular interest in this HPC context with slurm.

slurm and snow

Having introduced `snow`, `slurm` and `r`, we would like to combine them.

However, there are problems:

- `snow` has a master/worker paradigm yet `slurm` launches its nodes symmetrically,
- `slurm`'s `srun` has limits in spawning jobs
- with `srun`, we cannot communicate the number of nodes 'dynamically' into the script: `snow`'s cluster creation needs a hardwired number of nodes

slurm and snow solution

`snow` solves the master / worker problem by auto-discovery upon startup. The package contains two internal files `RMPISNOW` and `RMPISNOWprofile` that use a combination of shell and R code to determine the node idendity allowing it to switch to master or worker functionality.

We can reduce the same problem to this for our R script:

```
mpirank <- mpi.comm.rank(0)
if (mpirank == 0) {                     # are we the master ?
    makeMPIcluster()
} else {                                # or are we a slave ?
    sink(file="/dev/null")
    slaveLoop(makeMPImaster())
    q()
}
```

slurm and snow solution

For example

```
1  #!/usr/bin/env r
2
3  suppressMessages(library(Rmpi))
4  suppressMessages(library(snow))
5
6  mpirank <- mpi.comm.rank(0)
7  if (mpirank == 0) {
8      cat("Launching master, mpi rank=", mpirank, "\n")
9      makeMPIcluster()
10 } else {                                  # or are we a slave ?
11     cat("Launching slave with, mpi rank=", mpirank, "\n")
12     sink(file="/dev/null")
13     slaveLoop(makeMPImaster())
14     mpi.finalize()
15     q()
16 }
17
18 stopCluster(cl)
```

slurm and snow solution

The example creates

```
$ orterun -H ron,joe,tony,mccoy -n 4 mpiSnowSimple.r

Launching slave 2
Launching master 0
Launching slave 1
Launching slave 3
```

and we see that $N - 1$ workers are running with one instance running as the coordinating manager node.

salloc for snow

The other important aspect is to switch to `salloc` (which will call `orterun`) instead of `srun`.

We can either supply the hosts used using the `-w` switch, or rely on the `slurm.conf` file.

But importantly, we can govern from the call how many instances we want running (and have neither the `srun` limitation requiring overcommitting nor the hard-coded `snow` cluster-creation size):

```
$ salloc -w ron,mccoy orterun -n 7 mpiSnowSimple.r
```

We ask for a `slurm` allocation on the given hosts, and instruct Open MPI to run seven instances.

salloc for snow

```
1  #!/usr/bin/env r
2  suppressMessages(library(Rmpi))
3  suppressMessages(library(snow))
4  mpirank <- mpi.comm.rank(0)
5  if (mpirank == 0) {
6      cat("Launching master, mpi rank=", mpirank, "\n")
7      makeMPIcluster()
8  } else {                                  # or are we a slave ?
9      cat("Launching slave with, mpi rank=", mpirank, "\n")
10     sink(file="/dev/null")
11     slaveLoop(makeMPImaster()); mpi.finalize(); q()
12 }
13
14 ## trivial main body, note how getMPIcluster() learns from the
15 ## launched cluster how many nodes are available
16 cl <- getMPIcluster()
17 clusterEvalQ(cl, options("digits.secs"=3)) ## show msecs
18 res <- clusterCall(cl, function() paste(format(Sys.time()),
19                                         Sys.info()["nodename"]))
20 print(do.call(rbind,res))
21 stopCluster(cl); mpi.quit()
```

salloc for snow

```
$ salloc -w ron,joe,tony orterun -n 7 /tmp/mpiSnowSimple

salloc: Granted job allocation 39
Launching slave with, mpi rank= 5
Launching slave with, mpi rank= 2
Launching slave with, mpi rank= 6
Launching master, mpi rank= 0
Launching slave with, mpi rank= 3
Launching slave with, mpi rank= 1
Launching slave with, mpi rank= 4
     [,1]
[1,] "2009-06-25 20:51:20.536 joe"
[2,] "2009-06-25 20:51:33.747 tony"
[3,] "2009-06-25 20:51:20.522 ron"
[4,] "2009-06-25 20:51:20.544 joe"
[5,] "2009-06-25 20:51:33.766 tony"
[6,] "2009-06-25 20:51:20.537 ron"
salloc: Relinquishing job allocation 39
```

A complete example

```
cl <- NULL
mpirank <- mpi.comm.rank(0)
if (mpirank == 0) {
    cl <- makeMPIcluster()
} else {                                # or are we a slave?
    sink(file="/dev/null")
    slaveLoop(makeMPImaster())
    mpi.finalize(); q()
}
clusterEvalQ(cl, library(RDieHarder))
res <- parLapply(cl, c("mt19937","mt19937_1999",
          "mt19937_1998", "R_mersenne_twister"),
         function(x) {
           dieharder(rng=x, test="operm5",
           psamples=100, seed=12345)  })
stopCluster(cl)
print(do.call(rbind,lapply(res,function(x) {x[[1]]})))
mpi.quit()
```

A complete example cont.

This uses `RDieHarder` to test four Mersenne-Twister implementations at once.

A simple analysis shows the four charts and prints the four *p*-values:

```
pdf("/tmp/snowRDH.pdf")
lapply(res, function(x) plot(x))
dev.off()

print( do.call(rbind,
               lapply(res, function(x) { x[[1]] } )))
```

A complete example cont.

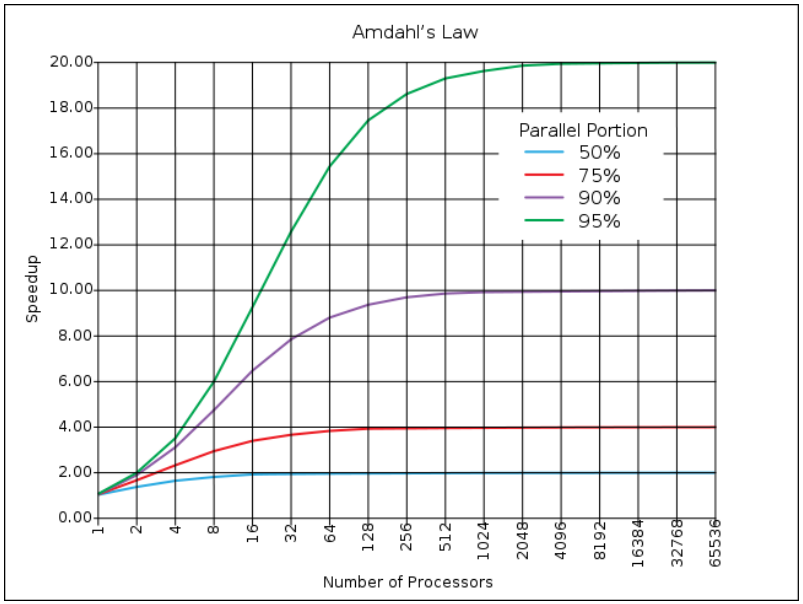
```
$ salloc -w ron,joe orterun -n 5 snowRDieharder.r

salloc: Granted job allocation 10
             [,1]
[1,] 0.1443805247
[2,] 0.0022301018
[3,] 0.0001014794
[4,] 0.0061524281
sall: Relinquishing job allocation 10
```

Amdahl's Law: An upper bound to speed gains

An upper bound to expected gains by parallelization is provided by Amdahl's law which relates the *proportion* P of total running time which can realize a *speedup* S due to parallelization (using S nodes) to the expected net speedup:

$$\frac{1}{(1-P) + \frac{P}{S}}$$

e.g. for $P = 0.75$ and $S = 128$ we expect a net speedup of up to 3.9.



Source: `http://en.wikipedia.org/wiki/Amdahl's_law`

Best practices for Parallel Computing with R

Quoting from the Schmidberger et al pager:

- Communication is much slower than computation; minimize data transfer to and from workers, maximize remote computation.
- Random number generators require extra care. Special-purpose packages `rsprng` and `rlecuyer` are available; `snow` provides an integrated interface.
- R's lexical scoping, serializing functions and the environments they are defined in require care to avoid transmitting unnecessary data. Functions used in `apply`-like calls should be defined in the global environment, or in a package name space. `forever` can be helpful too,

Outline

Extending physical RAM limits

Two CRAN packages ease the analysis of *large* datasets.

- `ff` which maps R objects to files and is therefore only bound by the available filesystem space
- `bigmemory` which maps R objects to dynamic memory objects not managed by R

Both packages can use the `biglm` package for out-of-memory (generalized) linear models.

Also worth mentioning are the older packages `g.data` for delayed data assignment from disk, `filehash` which takes a slightly more database-alike view by 'attaching' objects that are still saved on disk, and `R.huge` which also uses the disk to store the data.

biglm

The `biglm` package operates on 'larger-than-memory' datasets by operating on 'chunks' of data at a time.

```
make.data <- function ... # see 'help(bigglm)'
dataurl <-
   "http://faculty.washington.edu/tlumley/NO2.dat"
airpoll <- make.data(dataurl, chunksize=150, \
   col.names=c("logno2","logcars","temp",\
   "windsp","tempgrad","winddir","hour","day"))
b <- bigglm(exp(logno2)~logcars+temp+windsp, \
            data=airpoll, family=Gamma(log), \
            start=c(2,0,0,0),maxit=10)
summary(b)
```

Both `lm()` and `glm()` models can be estimated (and updated) this way.

ff: Large Objects

`ff` won the UseR! 2007 'large datasets' competition. It has since undergone a complete rewrite for versions 2.0 and 2.1.

`ff` provide memory-efficient storage of R objects on disk, and fast access functions that transparently map these in pagesize chunks to main memory. Many native data types are supported.

`ff` is complex package with numerous options that offer data access that can be tailored to be extremely memory-efficient.

ff: Large Objects cont.

As a small example, consider

```
b <- 1000
n <- 100000
k <- 3
x <- ff(vmode="double", dim=c(b*n,k), \
        dimnames=list(NULL, LETTERS[1:k]))
lsos()
```

```
                 Type  Size  Rows Columns
x          ff_matrix  2088 1e+08       3
b            numeric    32 1e+00      NA
k            numeric    32 1e+00      NA
n            numeric    32 1e+00      NA
```

We see the matrix *x* has 100 million elements and three columns, yet occupies only 2088 bytes (essentially an external pointer and some meta-data).

ff: Large Objects cont.

We can use `ff` along with `biglm`:

```
ffrowapply({
    l <- i2 - i1 + 1
    z <- rnorm(l)
    for (i in 1:k)  x[i1:i2,i] <- z + rnorm(l)
}, X=x, VERBOSE=TRUE, BATCHSIZE=n)

form <- A ~ B + C
first <- TRUE
ffrowapply({
 if (first){
  first <- FALSE
  fit <- biglm(form,as.data.frame(x[i1:i2,,drop=FALSE]))
 } else
  fit <- update(fit,as.data.frame(x[i1:i2,,drop=FALSE]))
}, X=x, VERBOSE=TRUE, BATCHSIZE=n)
```

bigmemory

The `bigmemory` package is similar to `ff` as it allows allocation and access to memory managed by the operating system but 'outside' of the view of R (and optionally mapped to disk).

`bigmemory` implements locking and sharing which allows multiple R sessions on the same host to access a common (large) object managed by `bigmemory`.

```
> object.size( big.matrix(1000,1000, "double") )

[1] 372

> object.size( matrix(double(1000*1000), ncol=1000) )

[1] 8000112
```

To R, a `big.matrix` of 1000×1000 elements occupies only 372 bytes of memory. The actual size of 800 mb is allocated by the operating system, and R interfaces it via an 'external pointer' object.

bigmemory cont.

We can illustrate `bigmemory` use of `biglm`:

```
x <- matrix(unlist(iris), ncol=5)
colnames(x) <- names(iris)
x <- as.big.matrix(x)

silly.biglm <- biglm.big.matrix(Sepal.Length ~ \
        Sepal.Width + Species, data=x, fc="Species")
summary(silly.biglm)
```

As before, the memory use of the new 'out-of-memory' object is smaller than the actual dataset as the 'real' storage is outside of what the R memory manager sees.

This can of course be generalized to really large datasets and 'chunked' access.

Example

The recent ASA dataviz competition asked for a graphical summary of a huge dataset.

We are going to look at the entry by Jay Emerson and his student Michael Kane as it covers several of the packages we looked at here.

The data contains flight arrival and departure data for almost all commercial flights within the USA from October 1987 to April 2008.

There are almost 120 million records and 29 variables, with some recoding done by Emerson and Kane.

Example: Sequential data access

Task: For every plane, find the month of its earliest flight in the data set.

```
# Take one: Sequential
#
date()
numplanes <- length(unique(x[,"TailNum"])) - 1
planeStart <- rep(0, numplanes)
for (i in theseflights) {  ## theseflights is a sample
  y <- x[mwhich(x, "TailNum", i, 'eq'),
         c("Year", "Month"), drop=FALSE]  # Note this.
  minYear <- min(y[,"Year"], na.rm=TRUE)
  these <- which(y[,"Year"]==minYear)
  minMonth <- min(y[these,"Month"], na.rm=TRUE)
  planeStart[i] <- 12*minYear + minMonth
  cat("TailNum",i,minYear,minMonth,nrow(y),planeStart[i],"\n")
}
planeStart[planeStart!=0]
date()  ## approximately 9 hours on the Yale cluster
```

Example: Sequential data access

```
# Take two: foreach(), sequential:
#
require(foreach)
date()
planeStart <- foreach(i=theseflights, .combine=c) %dopar% {
  y <- x[mwhich(x, "TailNum", i, 'eq'),
         c("Year", "Month"), drop=FALSE]  # Note this.
  minYear <- min(y[,"Year"], na.rm=TRUE)
  these <- which(y[,"Year"]==minYear)
  minMonth <- min(y[these,"Month"], na.rm=TRUE)
  cat("TailNum",i, minYear, minMonth, nrow(y), planeStart[i], "\
      n")
  12*minYear + minMonth
}
planeStart
date()  ## time ?
```

Example: Sequential data access

```
# Take three: foreach() and multicore
#
# Master and four workers
#
library(doMC)
registerDoMC()
date()
planeStart <- foreach(i=theseflights, .combine=c) %dopar% {
  x <- attach.big.matrix(xdesc)
  y <- x[mwhich(x, "TailNum", i, 'eq'),
         c("Year", "Month"), drop=FALSE]  # Note this.
  minYear <- min(y[,"Year"], na.rm=TRUE)
  these <- which(y[,"Year"]==minYear)
  minMonth <- min(y[these,"Month"], na.rm=TRUE)
  rm(x); gc()
  12*minYear + minMonth
}
planeStart
date() ## now about 2.5 hours
```

Example: Sequential data access

```
# Take four: foreach() and snow / SOCK
#
# Master and three workers
#
library(doSNOW)
cl <- makeSOCKcluster(3)
registerDoSNOW(cl)
date()
planeStart <- foreach(i=theseflights, .combine=c) %dopar% {
  require(bigmemory)
  x <- attach.big.matrix(xdesc)
  y <- x[mwhich(x, "TailNum", i, 'eq'),
         c("Year", "Month"), drop=FALSE]   # Note this.
  minYear <- min(y[,"Year"], na.rm=TRUE)
  these <- which(y[,"Year"]==minYear)
  minMonth <- min(y[these,"Month"], na.rm=TRUE)
  12*minYear + minMonth
}
planeStart
stopCluster(cl)
date()  ## about 3.5 hours
```

Outline

Wrapping up

In this tutorial session, we covered

- *scripting* and automation using littler, Rscript and RPy
- *profiling* and tools for *visualising profiling* output
- gaining speed using *vectorisation*, *Ra* and *just-in-time* compilation
- even more speed via *compiled code* using tools like *inline* and *Rcpp*, and how to embed R in C++ programs
- running R code in *parallel*, explicitly and implicitly
- working with *large datasets* that exceed the available memory size

Wrapping up

Further questions ?

Two good resources are

- the mailing list `r-sig-hpc` on HPC with R,
- the `HighPerformanceComputing` task view on CRAN.

Further resources:

- (Some) scripts are at `http://dirk.eddelbuettel.com/code/hpcR/`
- Updated versions of the tutorial may appear at `http://dirk.eddelbuettel.com/presentations.html`

Do not hesitate to email me at `edd@debian.org`

Thank You!